

Simulation of Hubbard Models in the Era of Synthetic Gauge Field

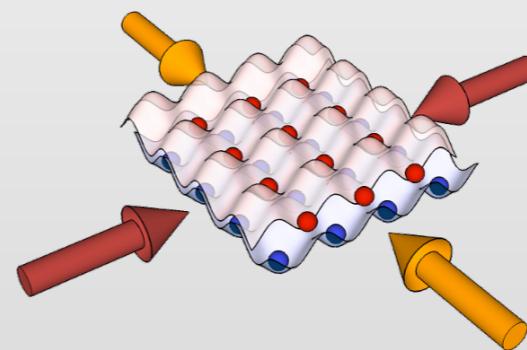
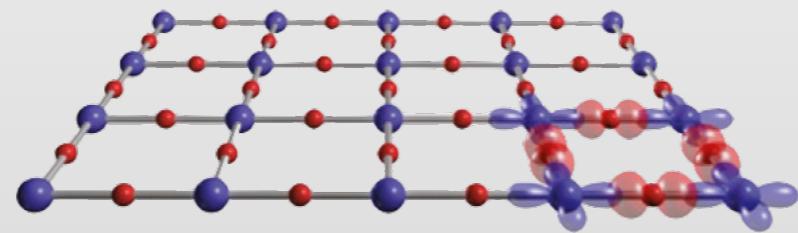
Lei Wang
Institute of Physics

Hubbard Model

$$\hat{H} = - \sum_{i,j,\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

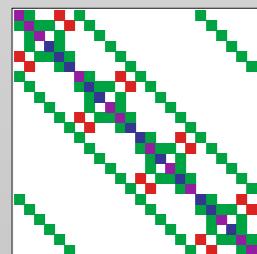
d-wave SC
Mott physics
Magnetism
BCS-BEC
...

Solid materials

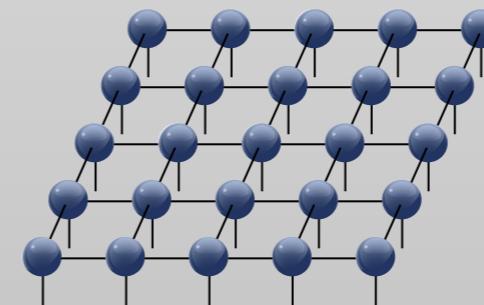


Optical lattices

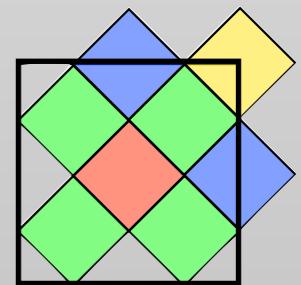
Algorithms for quantum many body systems



exact
diagonalization



tensor network
states



dynamical mean
field theories



better scaling

Iazzi and Troyer, PRB 2015
LW, Iazzi, Corboz and Troyer, PRB 2015
Liu and LW, PRB 2015
LW, Liu and Troyer, PRB 2016



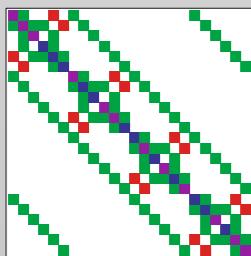
entanglement & fidelity

LW and Troyer, PRL 2014
LW, Liu, Imriška, Ma and Troyer, PRX 2015
LW, Shinaoka and Troyer, PRL 2015
Huang, Wang, LW and Werner, arXiv 2016



sign problem

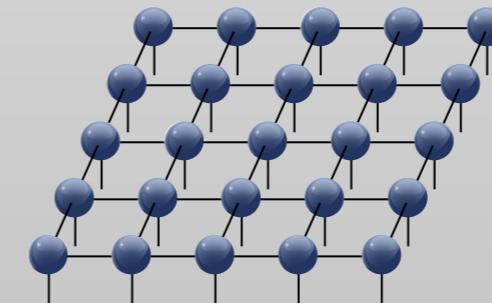
Huffman and Chandrasekharan, PRB 2014
Li, Jiang and Yao, PRB 2015
LW, Liu, Iazzi, Troyer and Harcos, PRL 2015
Wei, Wu, Li, Zhang and Xiang, PRL 2016



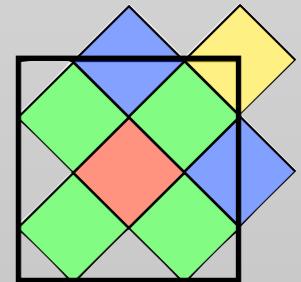
exact diagonalization



quantum Monte Carlo

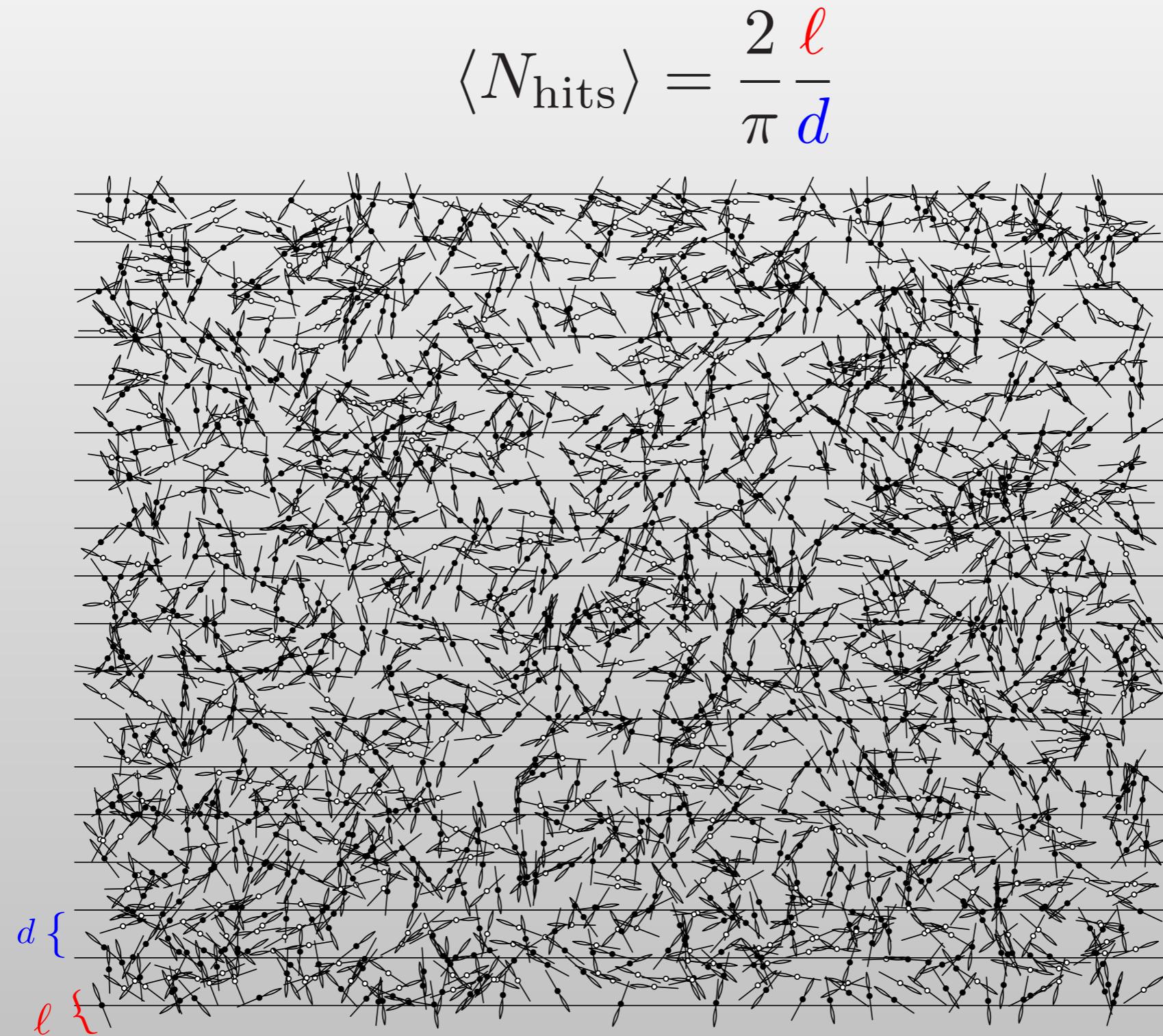


tensor network states



dynamical mean field theories

The first recorded Monte Carlo simulation



Buffon 1777

Statistical Mechanics:
Algorithms and Computations
Werner Krauth

Equation of State Calculations by Fast Computing Machines

NICHOLAS METROPOLIS, ARIANNA W. ROSENBLUTH, MARSHALL N. ROSENBLUTH, AND AUGUSTA H. TELLER,
Los Alamos Scientific Laboratory, Los Alamos, New Mexico

AND

EDWARD TELLER,* *Department of Physics, University of Chicago, Chicago, Illinois*

(Received March 6, 1953)

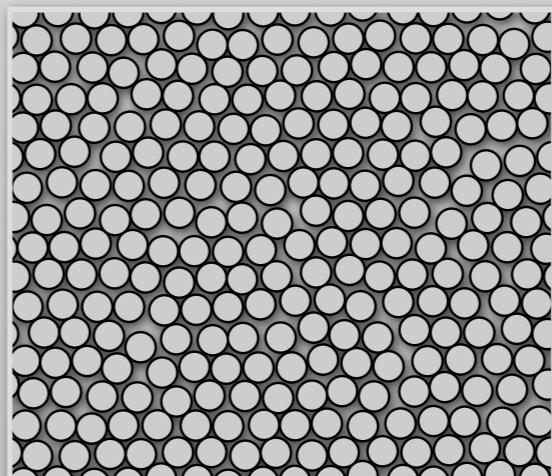
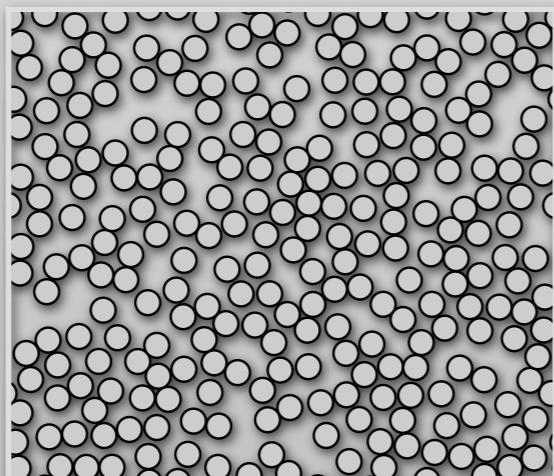
A general method, suitable for fast computing machines, for investigating such properties as equations of state for substances consisting of interacting individual molecules is described. The method consists of a modified Monte Carlo integration over configuration space. Results for the two-dimensional rigid-sphere system have been obtained on the Los Alamos MANIAC and are presented here. These results are compared to the free volume equation of state and to a four-term virial coefficient expansion.

I. INTRODUCTION

THE purpose of this paper is to describe a general method, suitable for fast electronic computing machines, of calculating the properties of any substance which may be considered as composed of interacting individual molecules. Classical statistics is assumed,

II. THE GENERAL METHOD FOR AN ARBITRARY POTENTIAL BETWEEN THE PARTICLES

In order to reduce the problem to a feasible size for numerical work, we can, of course, consider only a finite number of particles. This number N may be as high as several hundred. Our system consists of a square† con-

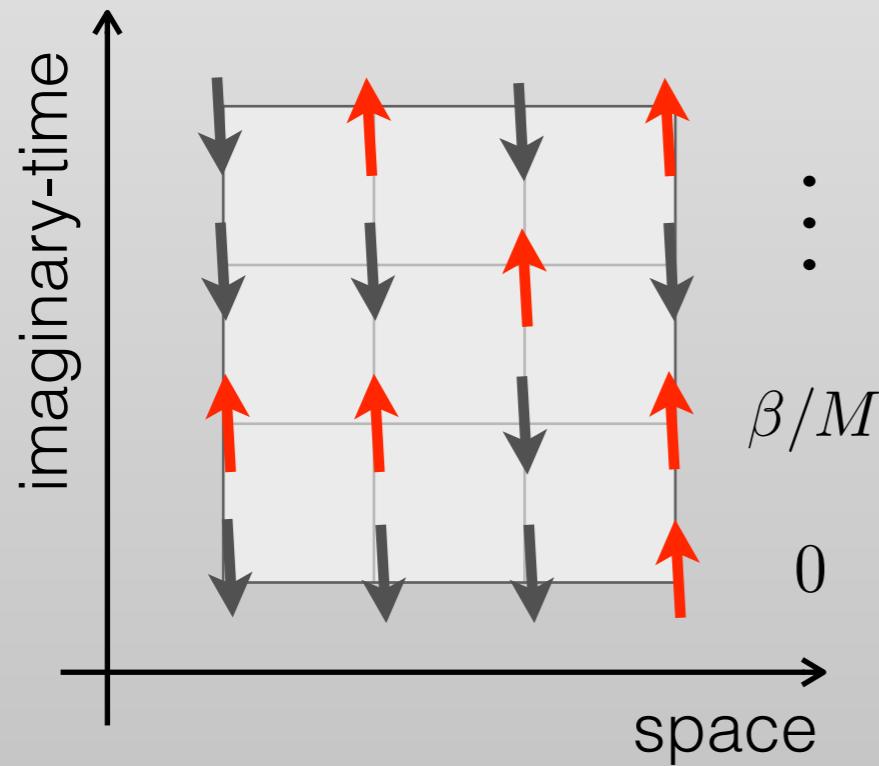


Quantum to classical mapping

$$Z = \text{Tr} \left(e^{-\beta \hat{H}} \right) \quad \hat{H} = \hat{H}_0 + \lambda \hat{H}_1$$

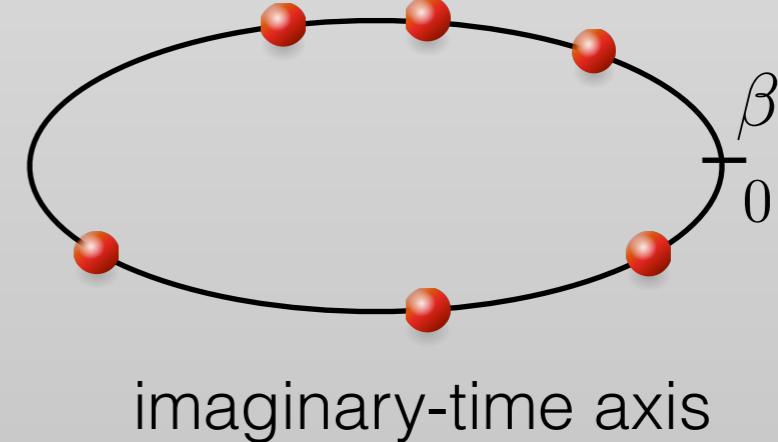
Trotterization

$$Z = \text{Tr} \left(e^{-\frac{\beta}{M} \hat{H}} \dots e^{-\frac{\beta}{M} \hat{H}} \right)$$



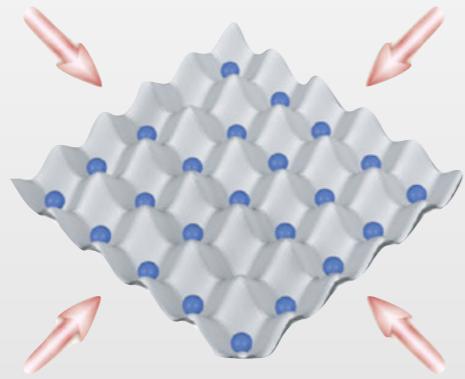
Diagrammatic approach

$$Z = \sum_{k=0}^{\infty} \lambda^k \int_0^{\beta} d\tau_1 \dots \int_{\tau_{k-1}}^{\beta} d\tau_k \times \text{Tr} \left[(-1)^k e^{-(\beta-\tau_k) \hat{H}_0} \hat{H}_1 \dots \hat{H}_1 e^{-\tau_1 \hat{H}_0} \right]$$



Beard and Wiese, 1996
Prokof'ev, Svistunov, Tupitsyn, 1996

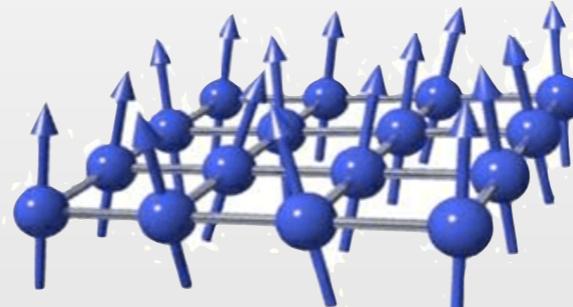
Diagrammatic approaches



bosons

World-line Approach

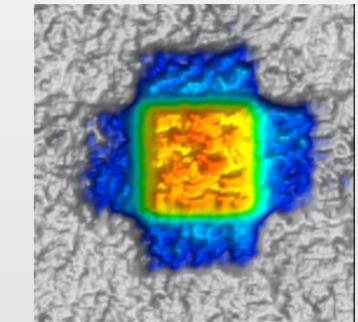
Prokof'ev et al, JETP, **87**, 310 (1998)



quantum spins

Stochastic Series Expansion

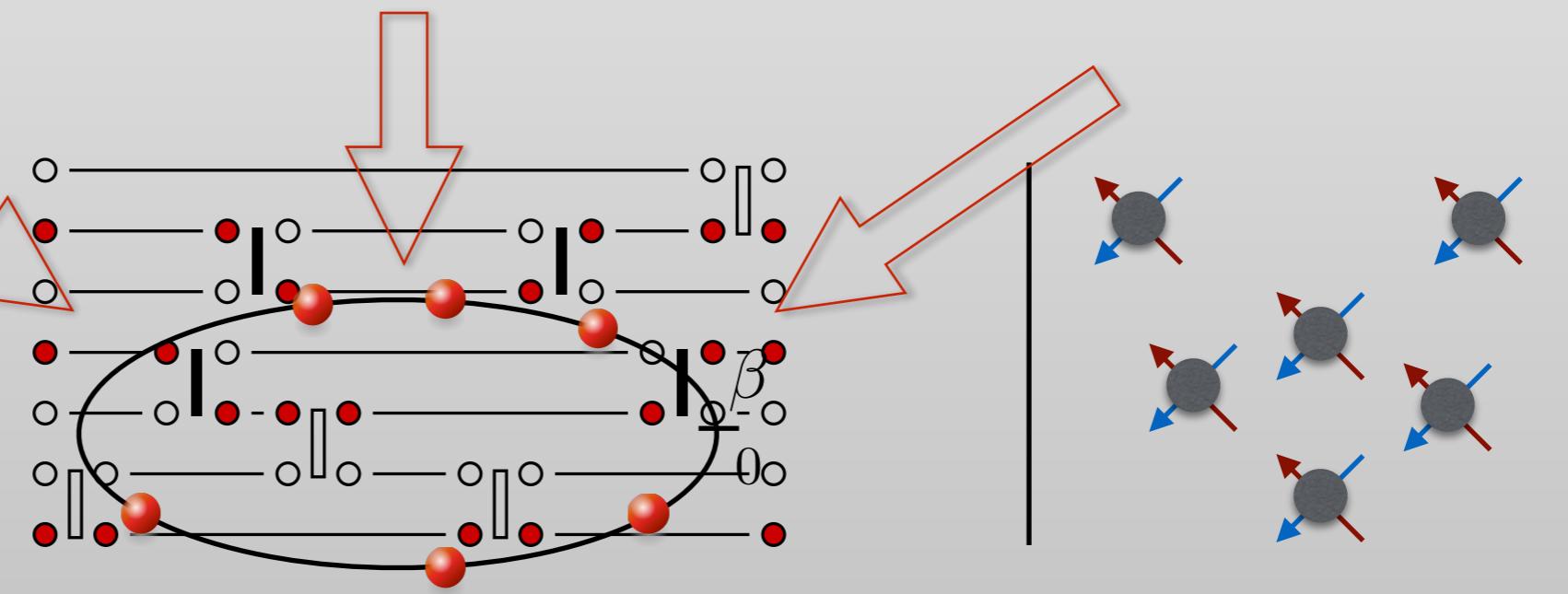
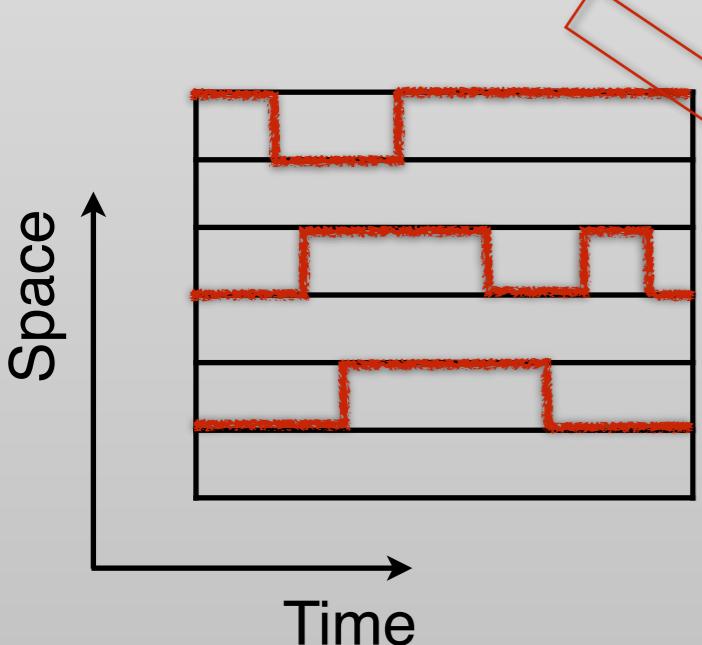
Sandvik et al, PRB, **43**, 5950 (1991)



fermions

Determinantal Methods

Gull et al, RMP, **83**, 349 (2011)



Aspects of QMC

- Unbiased method with statistical error more accurate if you run it longer
- Quite flexible in terms of temperature, dimension and range of interactions
- Frontier: compute quantum information quantities LW and Troyer, PRL 2014
LW, Liu, Imriška, Ma and Troyer, PRX 2015 LW, Shinaoka and Troyer, PRL 2015
- Can simulate millions of bosons/quantum spins on a PC, thousands of fermions on a cluster

...if there is no sign problem!

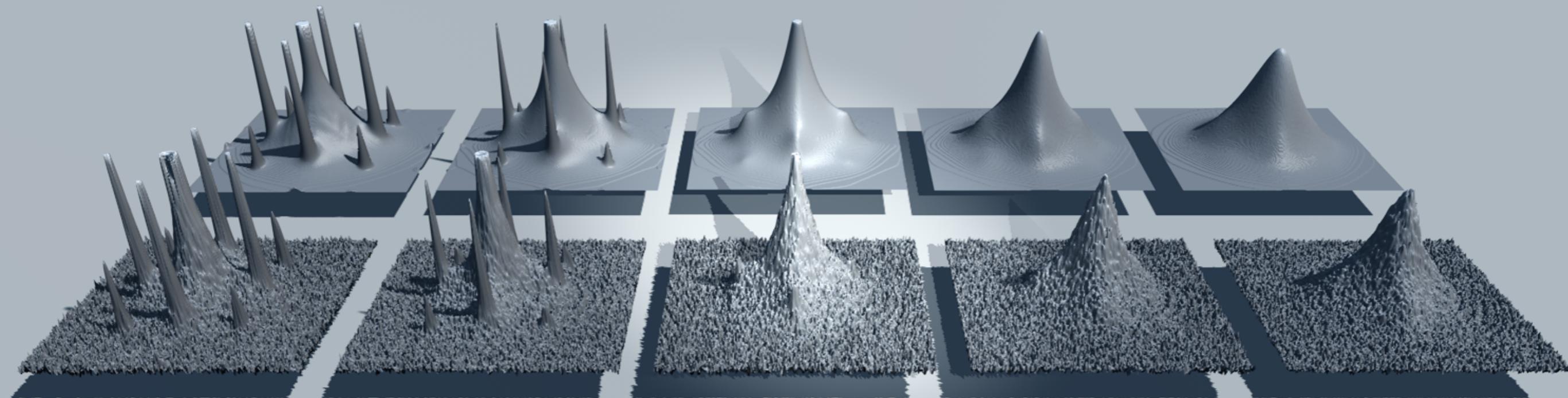
Calibrator

Model all details of the experiment

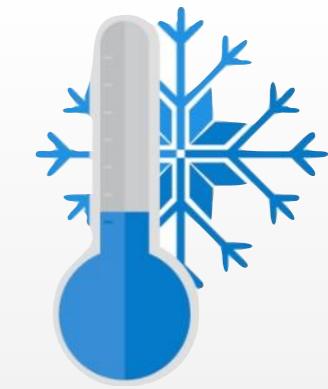
- ⌚ Accurate microscopic model (including the trap)
- ⌚ Actual size simulation (~300,000 bosons)
- ⌚ Calculate what the experiment should see

Time of flight image

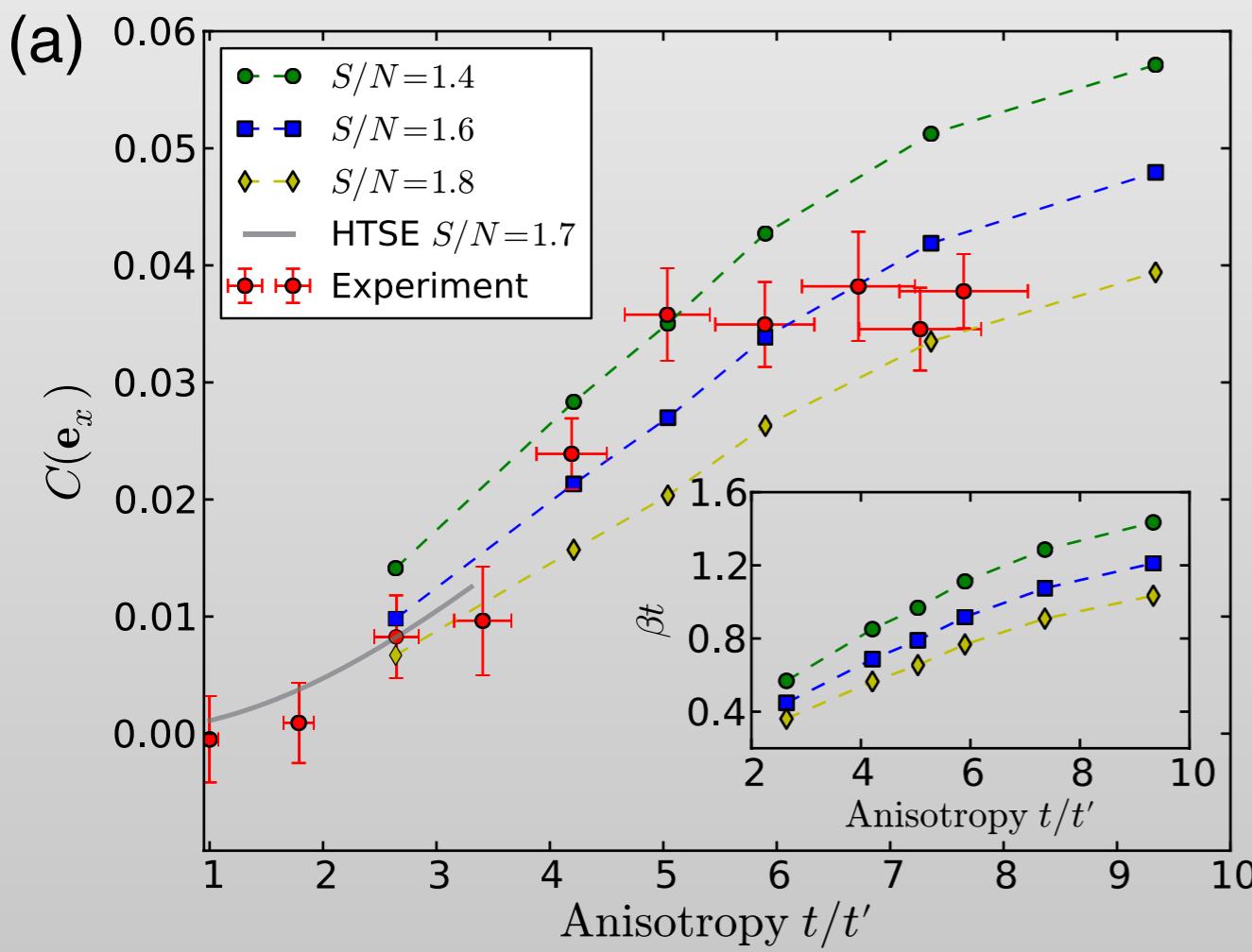
Trotzky, Pollet et al, Nat. Phys, 2010



Thermometer

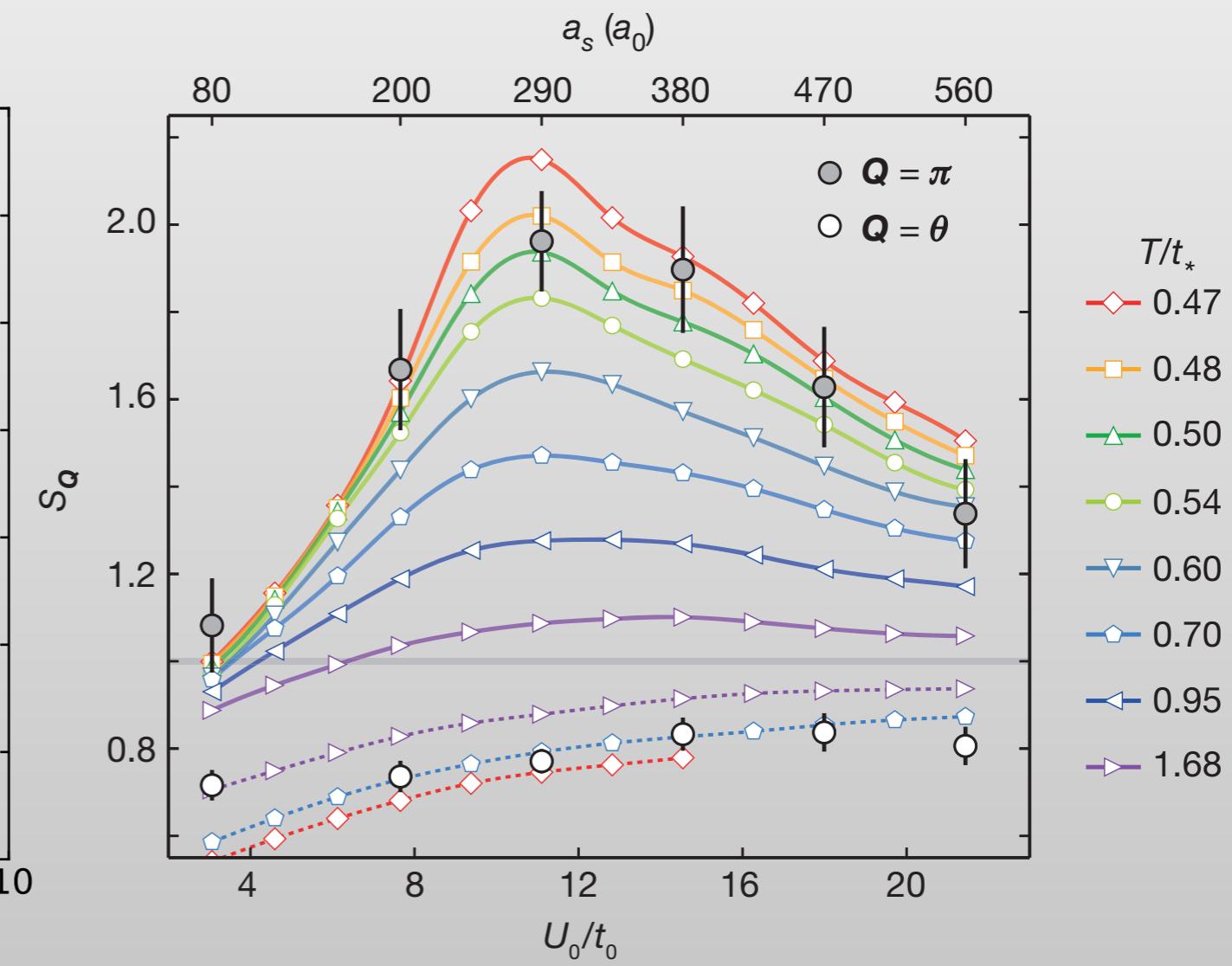


n.n. spin correlation



Imriska et al, PRL 2014

spin structure factor



Hart et al, Nature 2015

Theoretical guidance

Critical temperatures

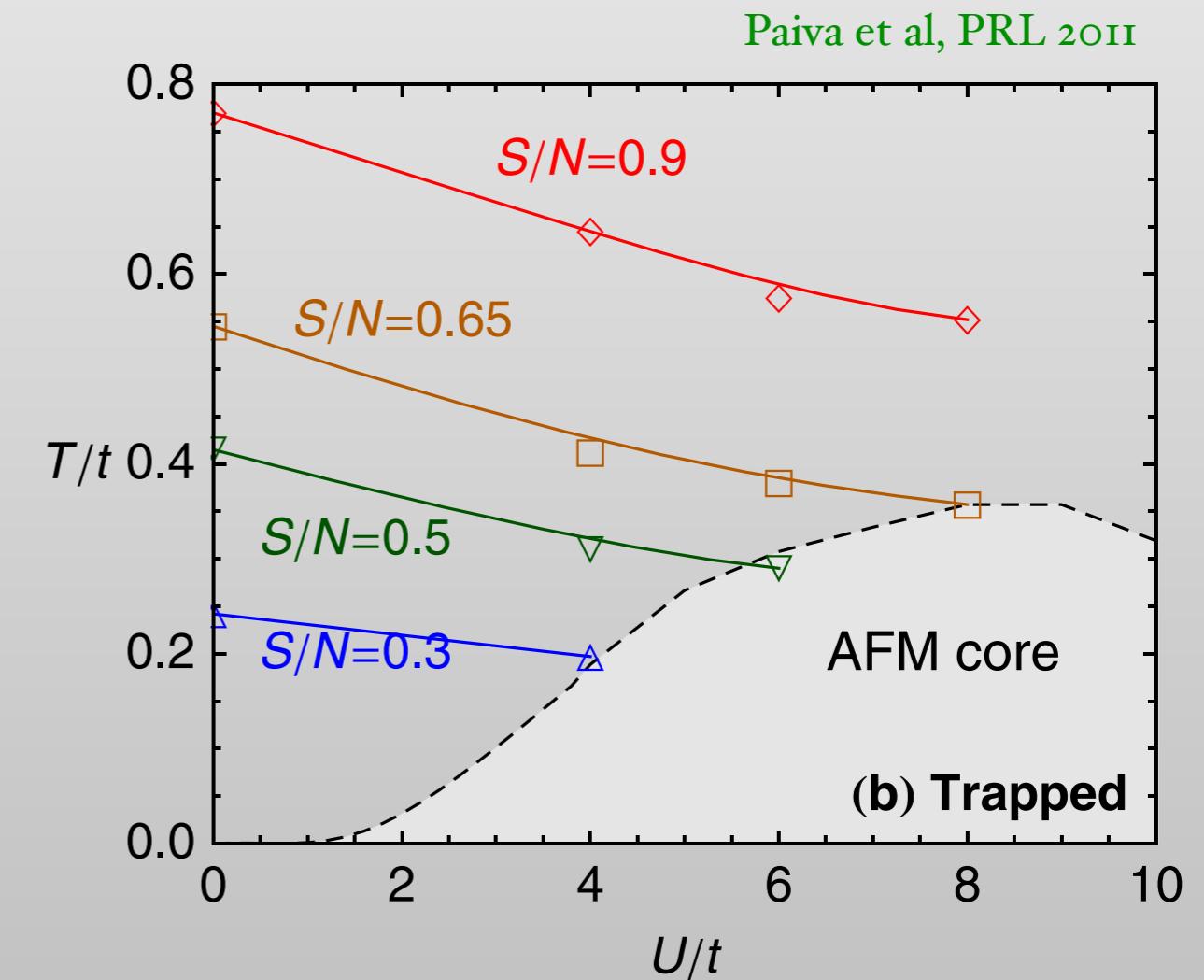
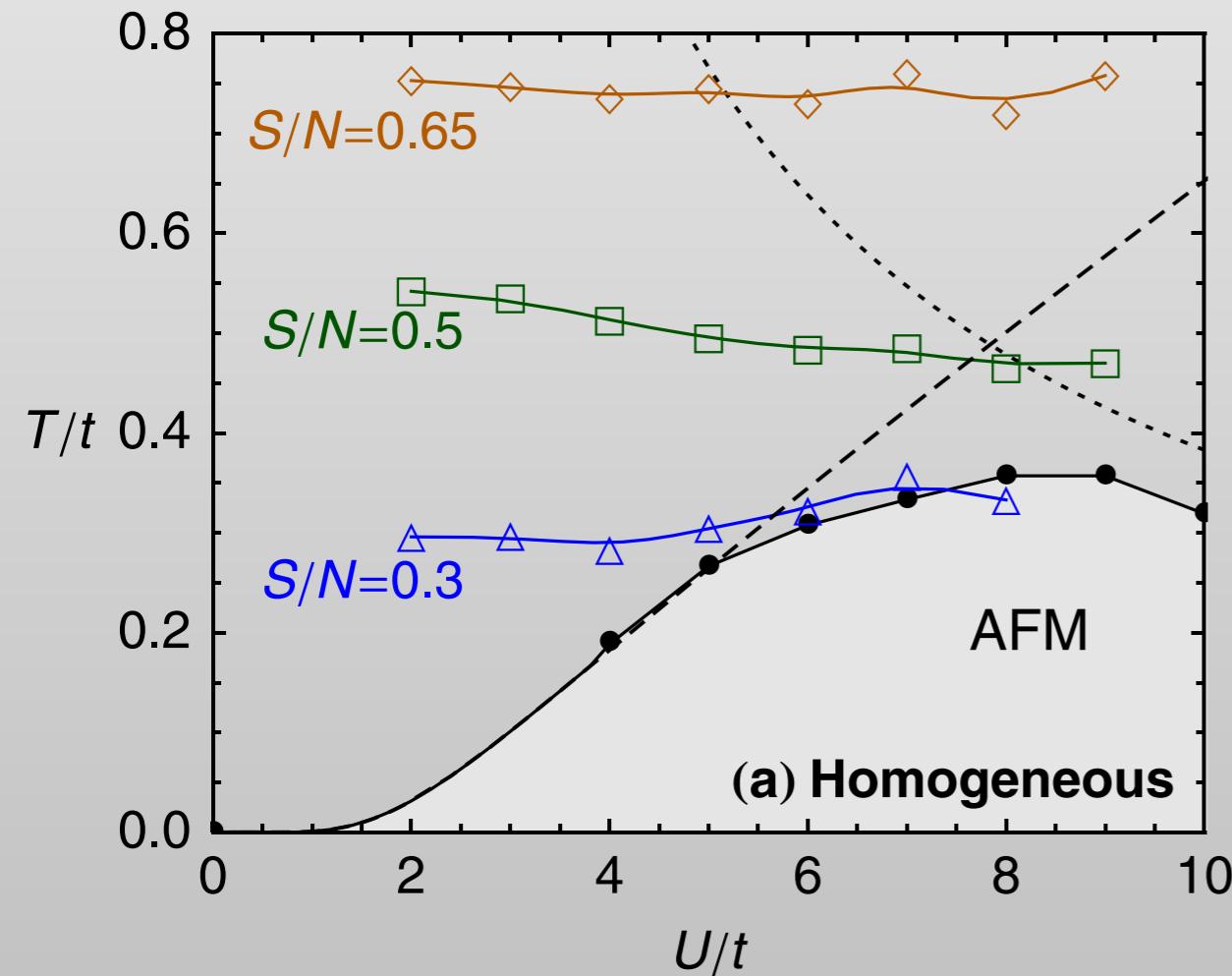
Staudt, Kent, Kozik...

Equation of states

Fuchs, LeBlanc, Rigol, Scalettar ...

Isentropic curves

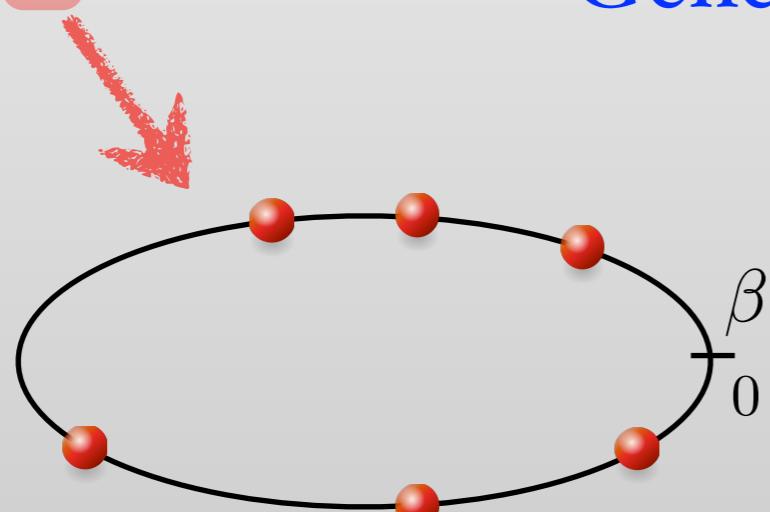
Pollet, Cai, Wang...



What about the sign problem ?

$$Z = \sum_{k=0}^{\infty} \int_0^{\beta} d\tau_1 \dots \int_{\tau_{k-1}}^{\beta} d\tau_k \text{Tr} \left[e^{-(\beta - \tau_k) \hat{H}_0} (-\lambda \hat{H}_1) \dots (-\lambda \hat{H}_1) e^{-\tau_1 \hat{H}_0} \right]$$

$$= \sum_{k=0}^{\infty} \sum_{\mathcal{C}_k} w(\mathcal{C}_k)$$



Is it all positive ?

General solution implies P=NP ! Troyer and Wiese, 2005



Bosons: no sign problem if there is **no frustration**

✓ QMC works for any filling, any lattice and any interactions

How about fermions ?

$$Z = \sum_{k=0}^{\infty} \int_0^{\beta} d\tau_1 \dots \int_{\tau_{k-1}}^{\beta} d\tau_k \text{Tr} \left[e^{-(\beta-\tau_k)\hat{H}_0} (-\lambda \hat{H}_1) \dots (-\lambda \hat{H}_1) e^{-\tau_1 \hat{H}_0} \right]$$

Rubtsov et al, PRB 2005 Gull et al, RMP 2011

$$= \sum_{k=0}^{\infty} \sum_{\mathcal{C}_k} w(\mathcal{C}_k) \xrightarrow{\quad} \det \begin{pmatrix} \text{Noninteracting} \\ \text{Green's functions} \end{pmatrix}_{k \times k}$$

$$\langle k \rangle \sim \beta \lambda N, \text{ scales as } \mathcal{O}(\beta^3 \lambda^3 N^3)$$



**LCT-QMC
Methods**

Rombouts, Heyde and Jachowicz, PRL 1999
Iazzi and Troyer, PRB 2015 LW, Iazzi, Corboz and Troyer, PRB 2015

$$\det \left(I + \mathcal{T} e^{-\int_0^{\beta} d\tau H_{\mathcal{C}_k}(\tau)} \right)_{N \times N}$$

thus achieving $\mathcal{O}(\beta \lambda N^3)$ scaling!

Fermion sign problem

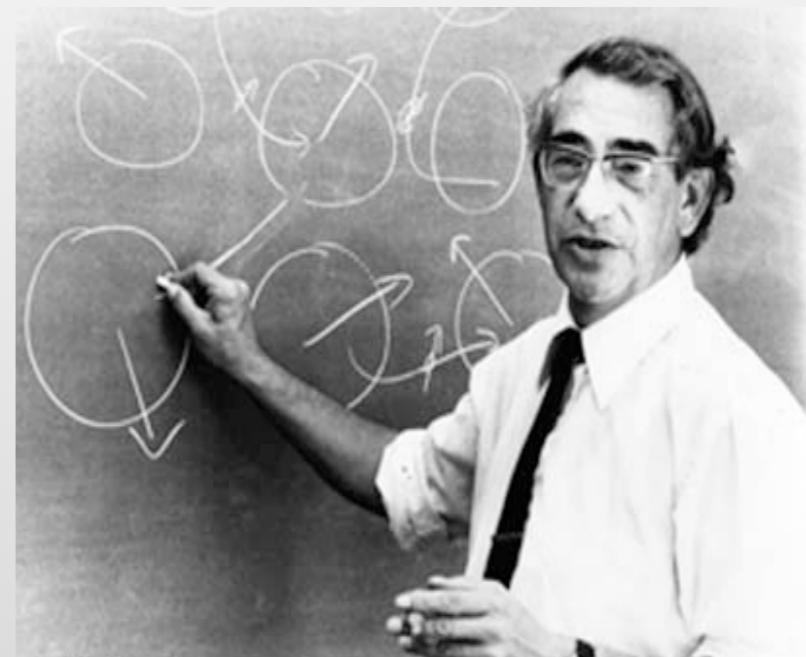
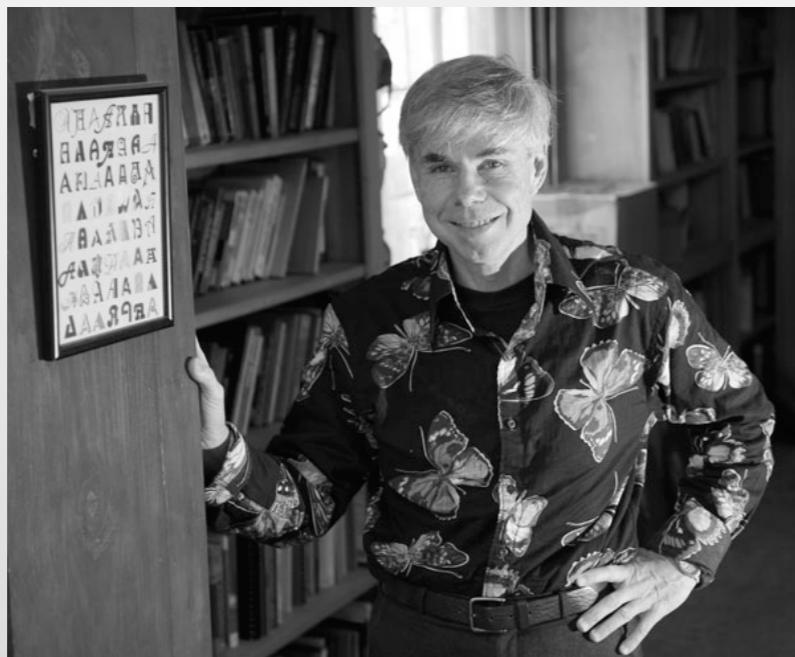
Spinful fermions: no sign problem thanks to
the time-reversal symmetry

$$M_{\uparrow} = M_{\downarrow}^*$$

$$\begin{aligned} w(\mathcal{C}_k) &= \det M_{\uparrow} \times \det M_{\downarrow} \\ &= |\det M_{\uparrow}|^2 \geq 0 \end{aligned}$$

Lang et al, Phys. Rev. C, 1993
Koonin et al, Phys. Rep., 1997
Hands et al, EPJC, 2000
Wu et al, PRB, 2005

- ✓ Attractive interaction at any filling on any lattice
- ✓ Repulsive interaction at half-filling on bipartite lattices
- ✓ Gauge fields are not impossible for fermions !



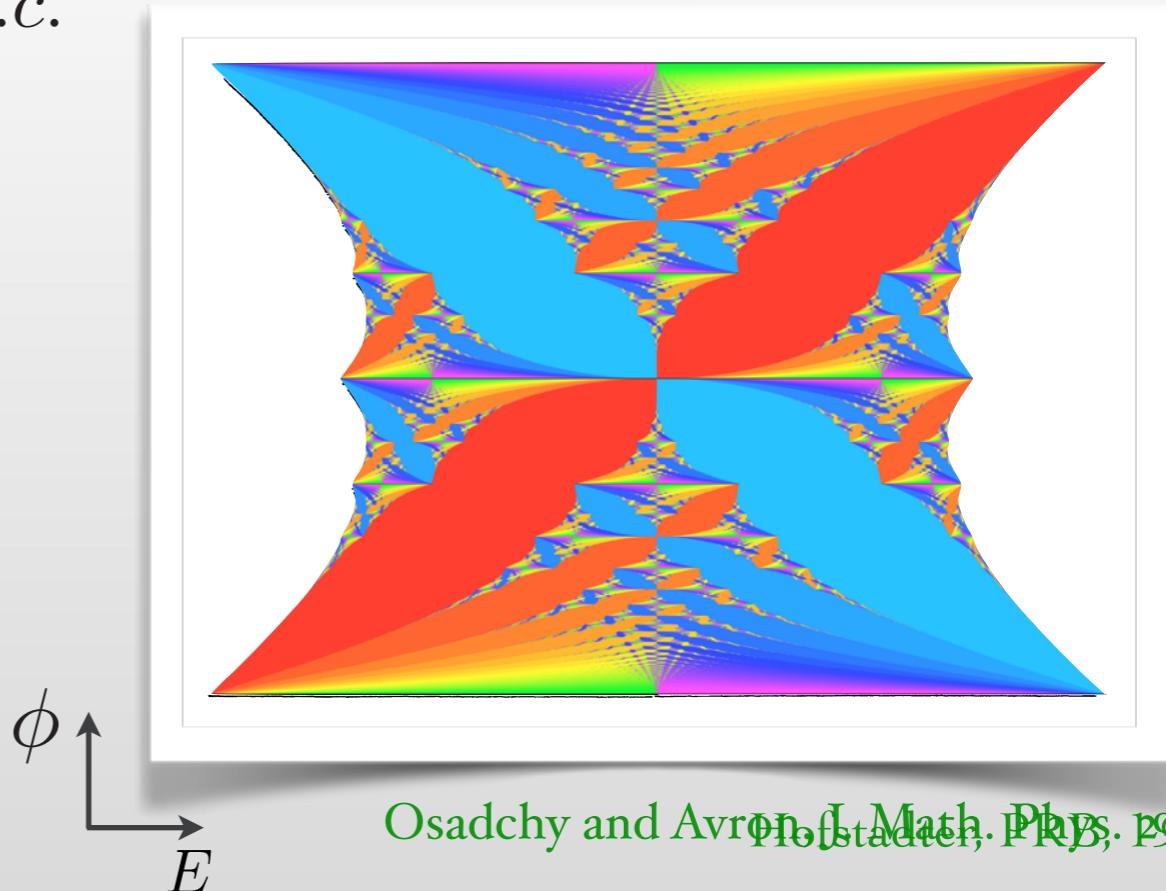
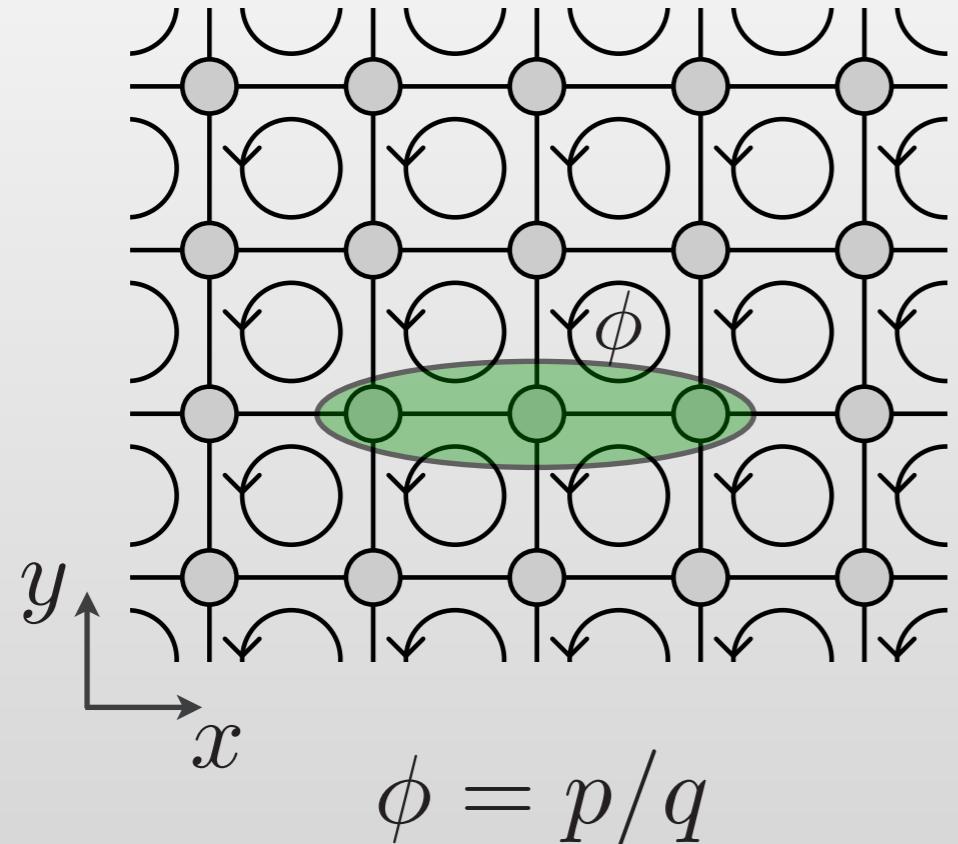
Hofstadter-Hubbard Model

when topology meets interaction

Wang, Hung and Troyer, PRB, 2014

Hofstadter Model

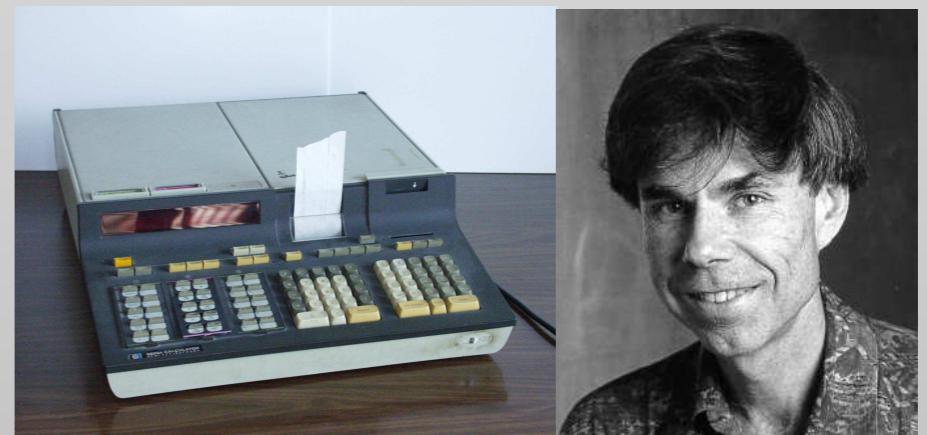
$$\hat{H} = \sum_{x,y} \hat{c}_{x+1,y}^\dagger \hat{c}_{x,y} + e^{i2\pi x\phi} \hat{c}_{x,y+1}^\dagger \hat{c}_{x,y} + h.c.$$



Thouless, Kohmoto, Nightingale and den Nijs, 1982

Chern number of the n-th gap is given by the Diophantine equation

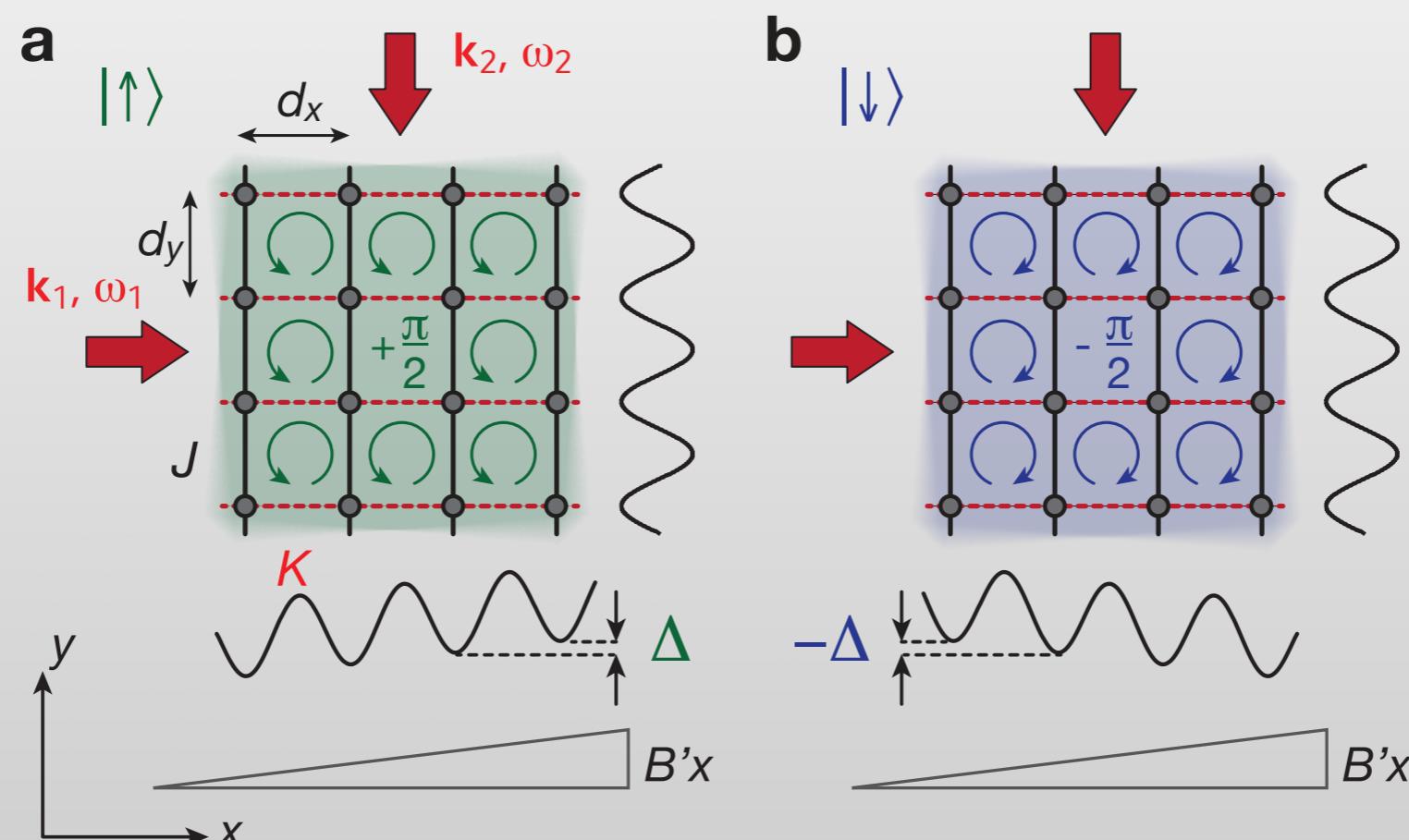
$$n = qs + pC$$



Time-Reversal Invariant Fluxes

Opposite fluxes for the two spin species

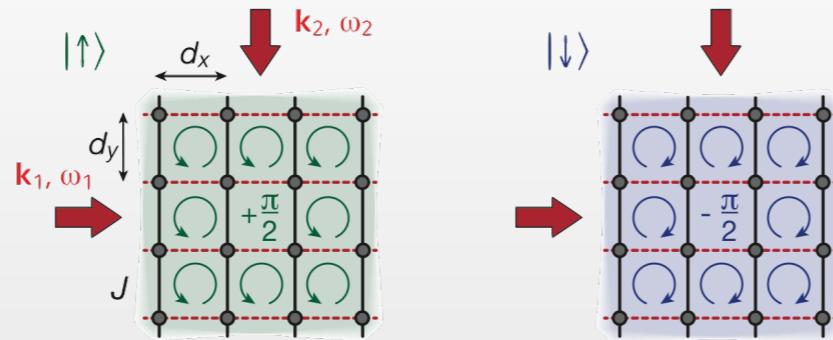
Aidelsburger et al, PRL 2013



Quantum Spin Hall Insulator
if load fermions into the lowest band

cf Miyake et al, PRL 2013 Kennedy et al, PRL 2013
and experiments in NIST, Hamburg ...

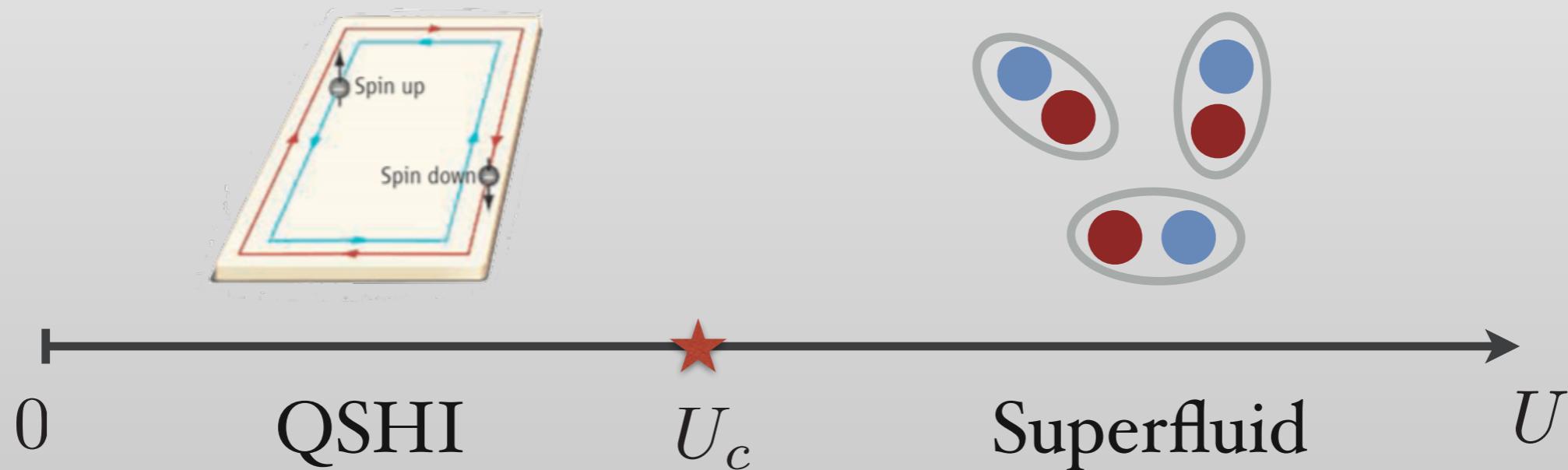
Hofstadter-Hubbard Model



Aidelsburger et al, PRL 2013
Miyake et al, PRL 2013
Kennedy et al, PRL 2013

$$\hat{H} = \hat{H}_\uparrow(\phi) + \hat{H}_\downarrow(-\phi) - U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

cf. same fluxes
Zhai et al, PRL 2010
cf. repulsive interaction
Cocks et al, PRL 2012

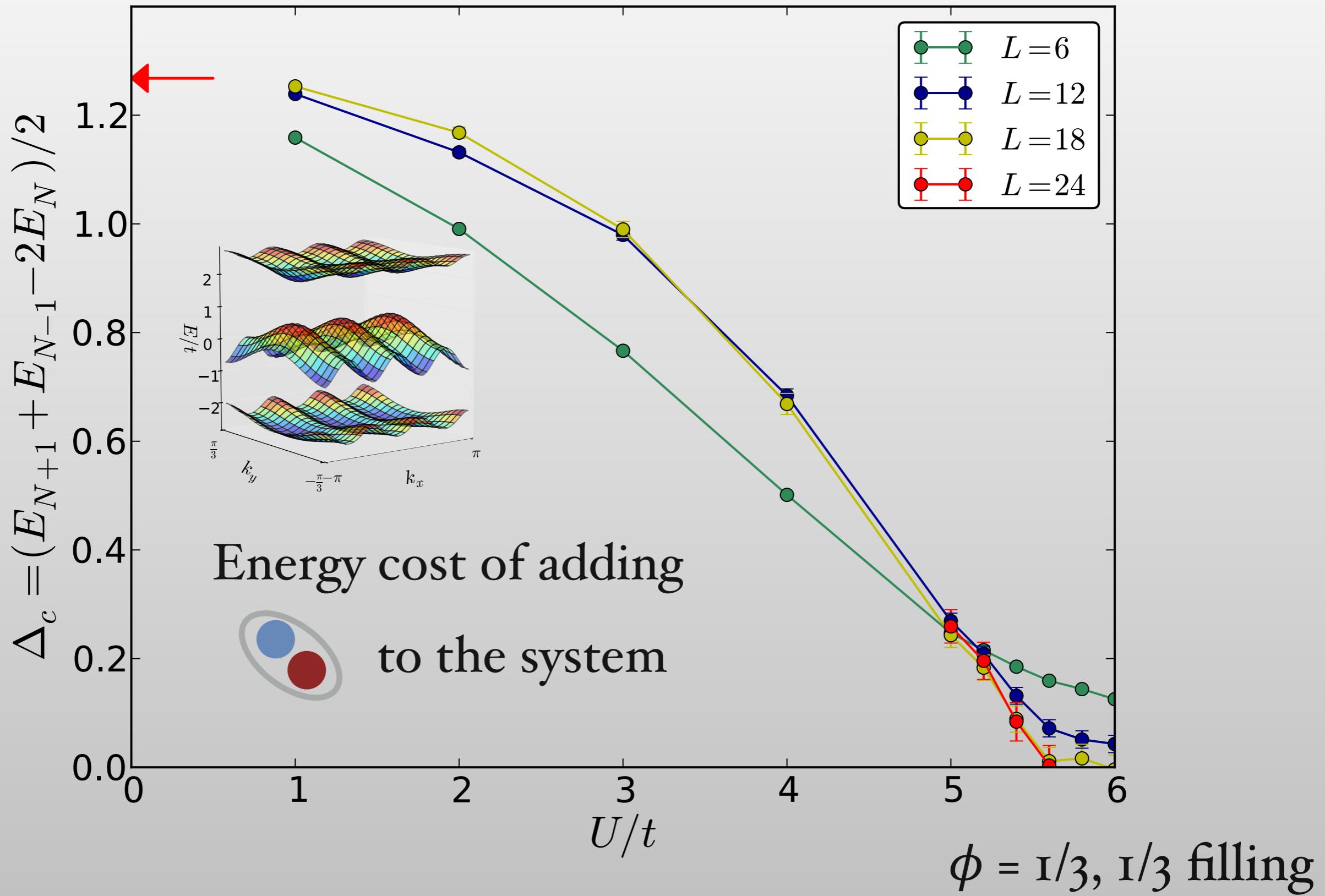


What's the topological signature of the transition ?

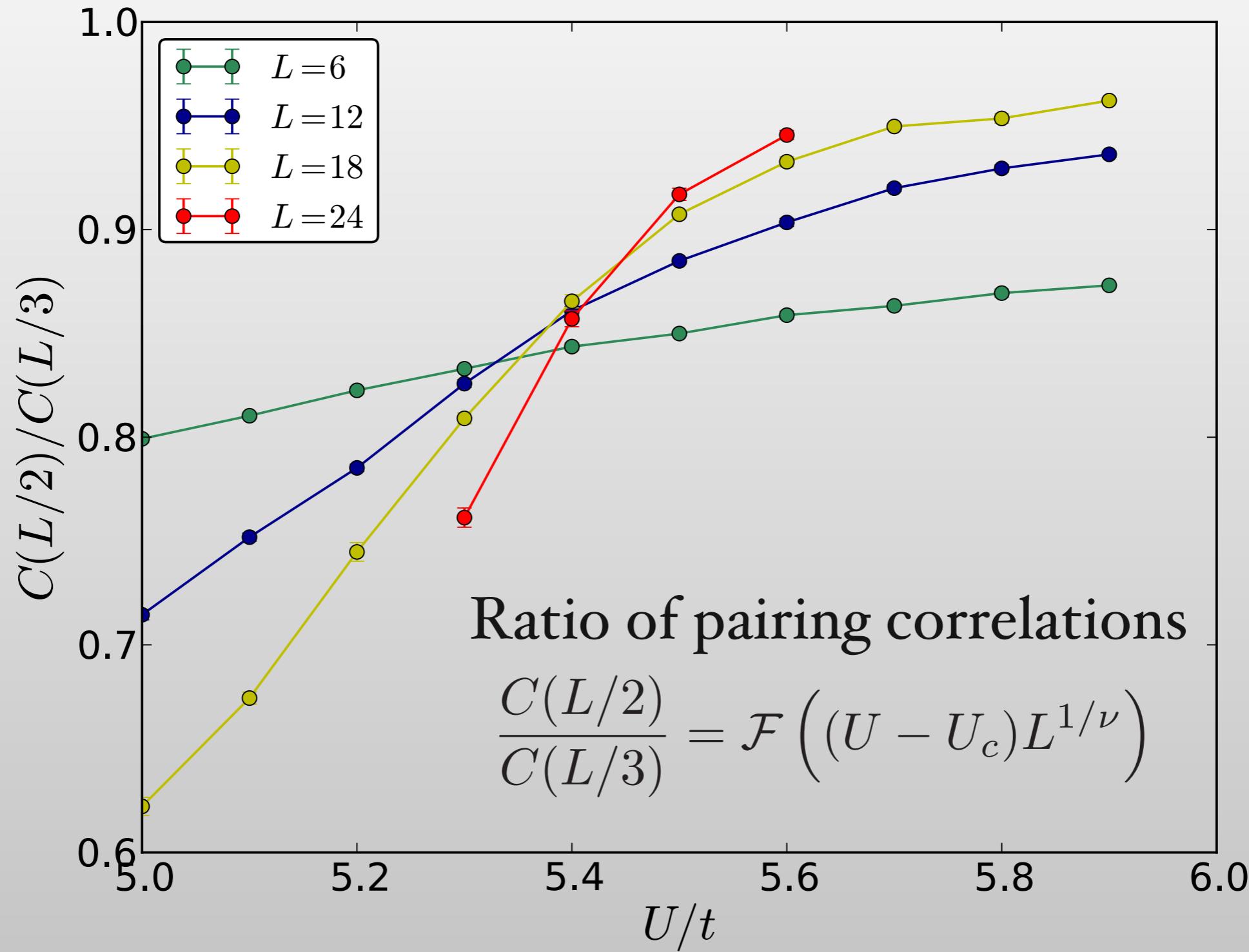
LW, Hung and Troyer, PRB 2014

Locate the transition point

LW, Hung and Troyer, PRB 2014



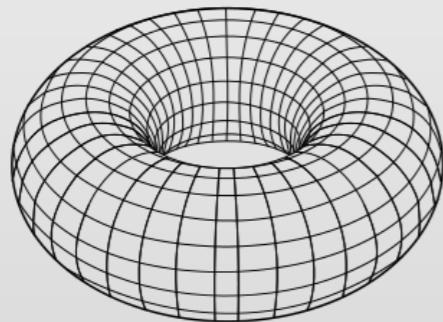
Locate the transition point



What can we say about topology ?

Niu, Thouless, Wu, 1985 Sheng et al, 2006

Twisted boundary conditions

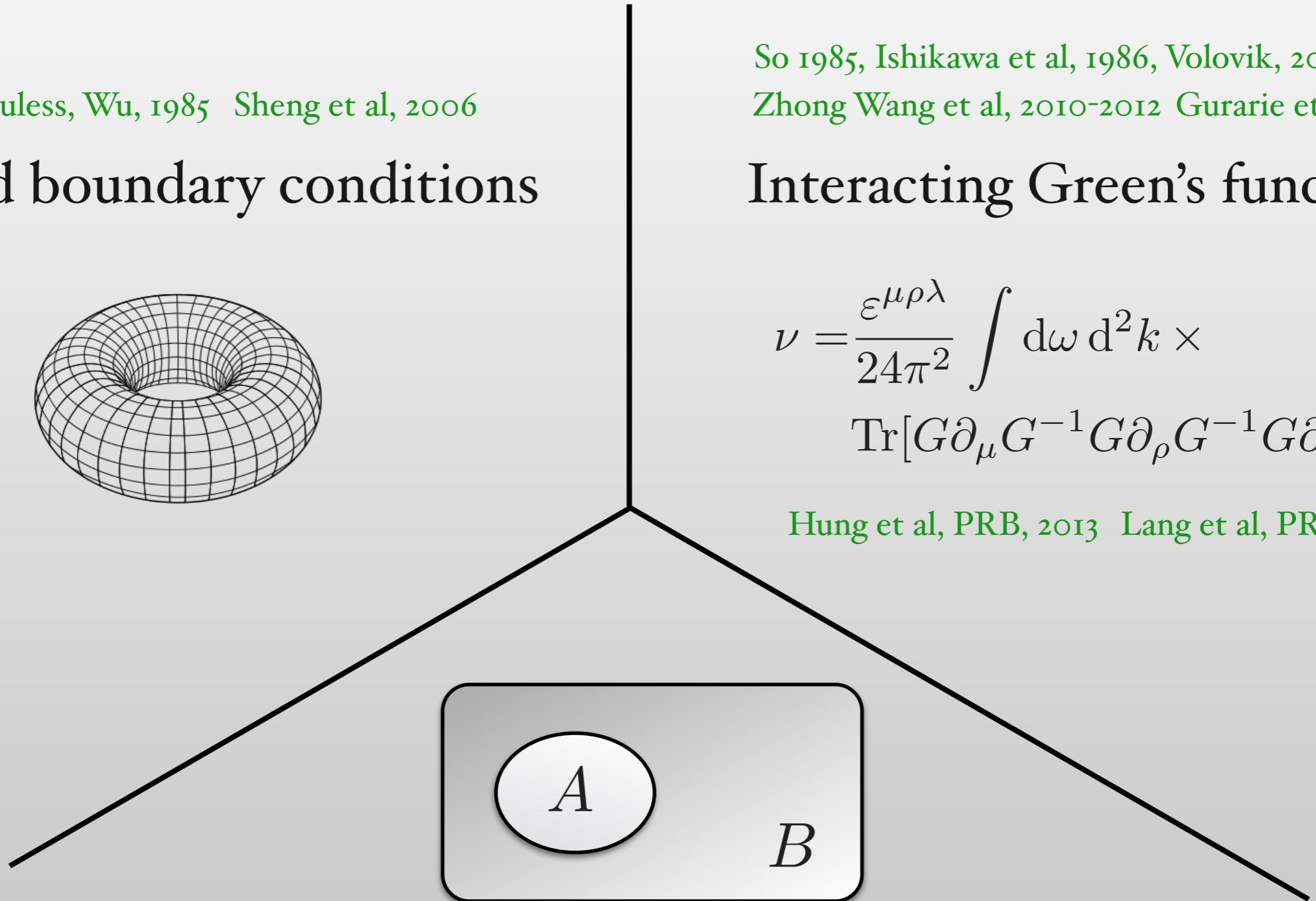


So 1985, Ishikawa et al, 1986, Volovik, 2003
Zhong Wang et al, 2010-2012 Gurarie et al, 2011

Interacting Green's function

$$\nu = \frac{\varepsilon^{\mu\rho\lambda}}{24\pi^2} \int d\omega d^2k \times \\ \text{Tr}[G\partial_\mu G^{-1}G\partial_\rho G^{-1}G\partial_\lambda G^{-1}]$$

Hung et al, PRB, 2013 Lang et al, PRB, 2013



Turner et al, 2010 Assaad et al, 2014 Da Wang et al, 2015
Entanglement entropy & spectra

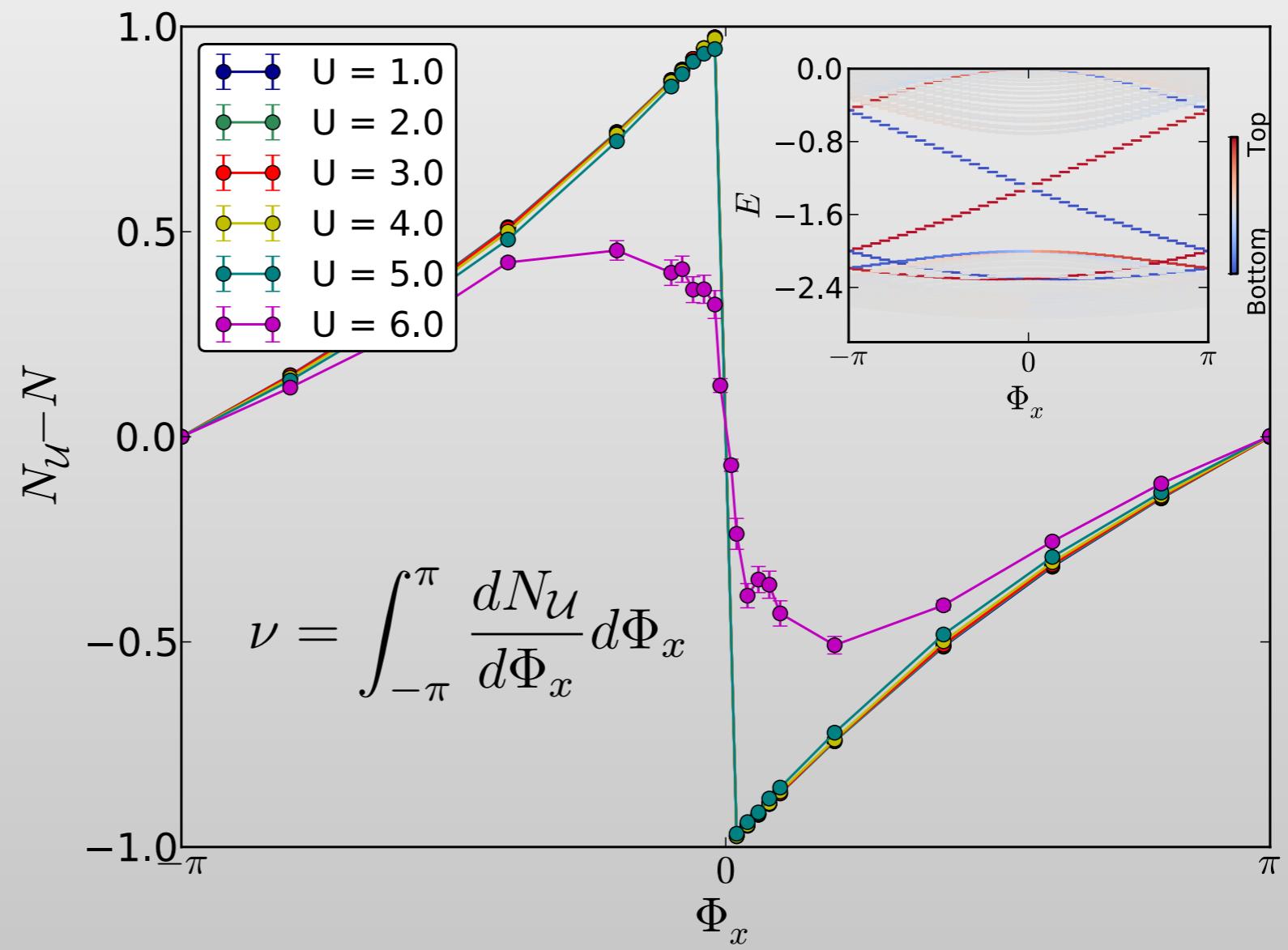
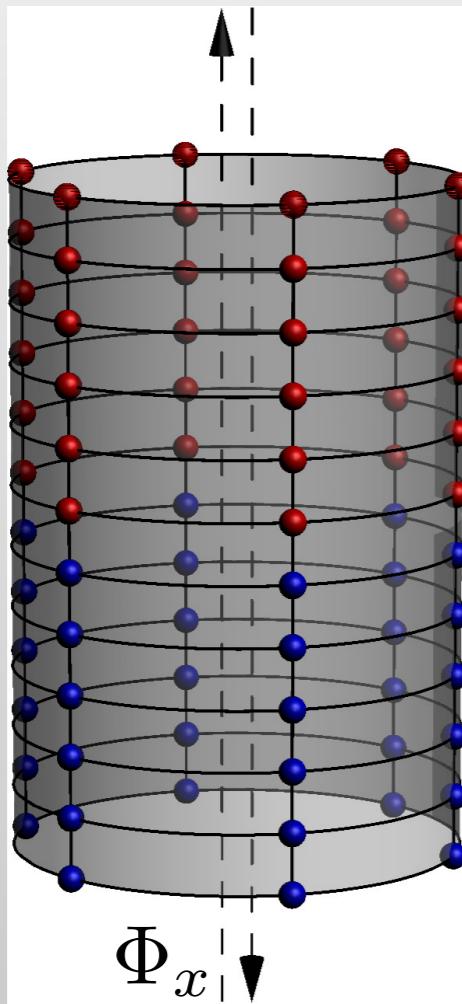
Topological Pumping

Laughlin, PRB 1981 Thouless, PRB 1983

LW, Hung and Troyer, PRB 2014

Flux insertion pumps quantized particle in the QSHI

$N_{\mathcal{U}}$



May even be measured in the experiment!

What about the sign problem ?



Sign problem free: Kramers pairs due to the time-reversal symmetry

$$M_{\uparrow} = M_{\downarrow}^*$$

$$\begin{aligned} w(\mathcal{C}_k) &= \det M_{\uparrow} \times \det M_{\downarrow} \\ &= |\det M_{\uparrow}|^2 \geq 0 \end{aligned}$$

Lang et al, Phys. Rev. C, 1993
Koonin et al, Phys. Rep., 1997
Hands et al, EPJC, 2000
Wu et al, PRB, 2005



But, how about this ?

Spinless fermions $\hat{H} = \sum_{\langle i,j \rangle} -t \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right) + V \left(\hat{n}_i - \frac{1}{2} \right) \left(\hat{n}_j - \frac{1}{2} \right)$

$$w(\mathcal{C}_k) = \det M$$

Scalapino et al, PRB 1984 Gubernatis et al, PRB 1985
up to 8*8 square lattice and $T \geq 0.3t$

Meron cluster approach, Chandrasekharan and Wiese, PRL 1999
solves sign problem for $V \geq 2t$



Solutions !

PHYSICAL REVIEW B **89**, 111101(R) (2014)

Solution to sign problems in half-filled spin-polarized electronic systems

Emilie Fulton Huffman and Shailesh Chandrasekharan

Department of Physics, Duke University, Durham, North Carolina 27708, USA

(Received 19 December 2013; revised manuscript received 14 February 2014; published 12 March 2014)



PHYSICAL REVIEW B **91**, 241117(R) (2015)



Solving the fermion sign problem in quantum Monte Carlo simulations by Majorana representation

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(Received 27 August 2014; revised manuscript received 13 October 2014; published 30 June 2015)

PHYSICAL REVIEW B **91**, 235151 (2015)



Efficient continuous-time quantum Monte Carlo method for the ground state of correlated fermions

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(Received 12 January 2015; revised manuscript received 13 March 2015; published 30 June 2015)

PRL **115**, 250601 (2015)

PHYSICAL REVIEW LETTERS

week ending
18 DECEMBER 2015

Split Orthogonal Group: A Guiding Principle for Sign-Problem-Free Fermionic Simulations

Lei Wang,¹ Ye-Hua Liu,¹ Mauro Iazzi,¹ Matthias Troyer,¹ and Gergely Harcos²

¹*Theoretische Physik, ETH Zurich, 8093 Zurich, Switzerland*

²*Alfréd Rényi Institute of Mathematics, Reáltanoda utca 13-15., Budapest H-1053, Hungary*

Latest update

Wei, Wu, Li, Zhang, Xiang,
PRL 2016

A tale of open science

$$w(\mathcal{C}_k) \sim \det \left(I + \mathcal{T} e^{-\int_0^\beta d\tau H_{\mathcal{C}_k}(\tau)} \right)$$

Free fermions with an effective imaginary-time dependent Hamiltonian

Let real matrices $A_i = \begin{pmatrix} 0 & B_i \\ B_i^T & 0 \end{pmatrix}$

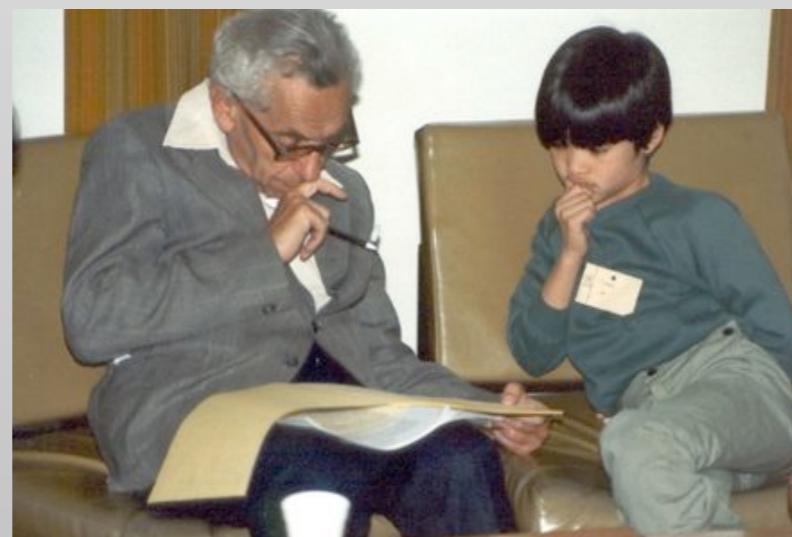
$$\text{then } \det(I + e^{A_1} e^{A_2} \dots e^{A_N}) \geq 0$$



[http://mathoverflow.net/questions/204460/
how-to-prove-this-determinant-is-positive](http://mathoverflow.net/questions/204460/how-to-prove-this-determinant-is-positive)

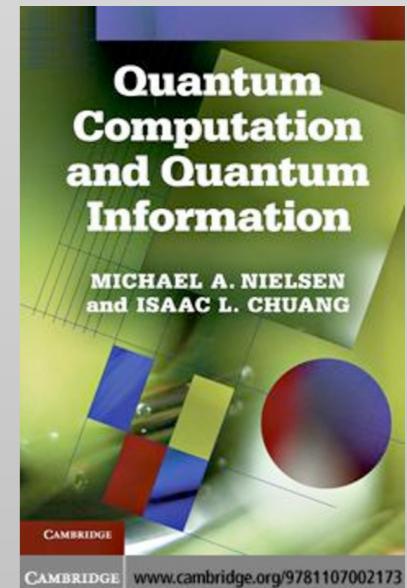
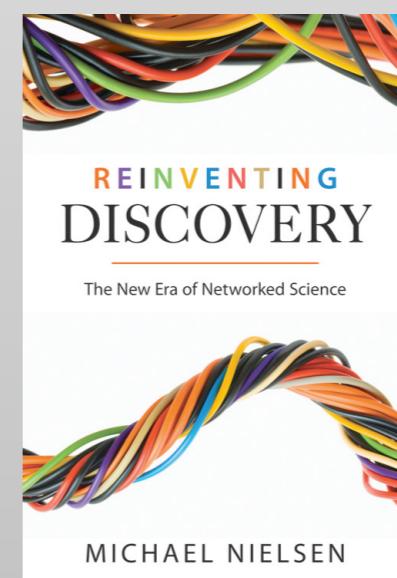


The conjecture was proved by Gergely Harcos and Terence Tao, with inputs from others



Tao and Paul Erdős in 1985

[https://terrytao.wordpress.com/2015/05/03/
the-standard-branch-of-the-matrix-logarithm/](https://terrytao.wordpress.com/2015/05/03/the-standard-branch-of-the-matrix-logarithm/)



A new “de-sign” principle

LW, Liu, Iazzi, Troyer and Harcos, PRL 2015

If $M^T \eta M = \eta$ where $\eta = \text{diag}(I, -I)$

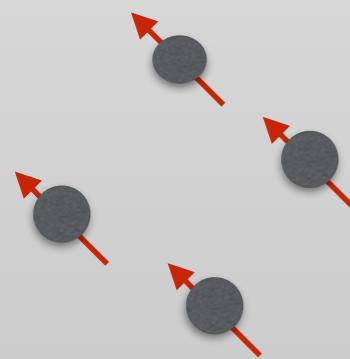
Then

$$\det \in IO(M, \eta)$$

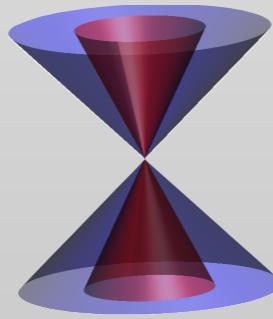
$\mathcal{T} e^{-\int_0^\beta d\tau H c_k(\tau)}$

has a orthogonal group
for each component !

$$\begin{array}{ccc} O^{+-}(n, n) & \equiv 0 & O^{++}(n, n) \\ \text{Yellow island} & & \text{Red island} \\ O^{--}(n, n) & \leq 0 & O^{-+}(n, n) \\ \text{Blue island} & & \text{Green island} \end{array} \geq 0$$



spinless fermions



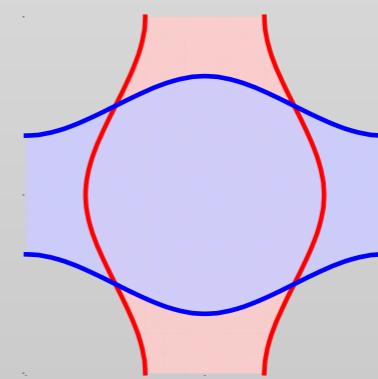
Liu and LW, PRB 2015

LW, Troyer, PRL 2014

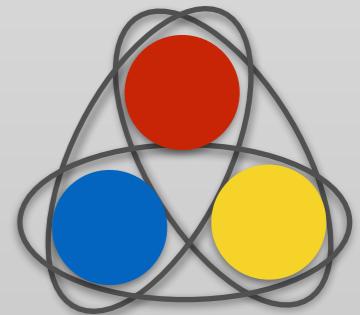
LW, Corboz, Troyer, NJP 2014

LW, Iazzi, Corboz, Troyer, PRB, 2015

LW, Liu and Troyer, arXiv 2016



spin nematicity



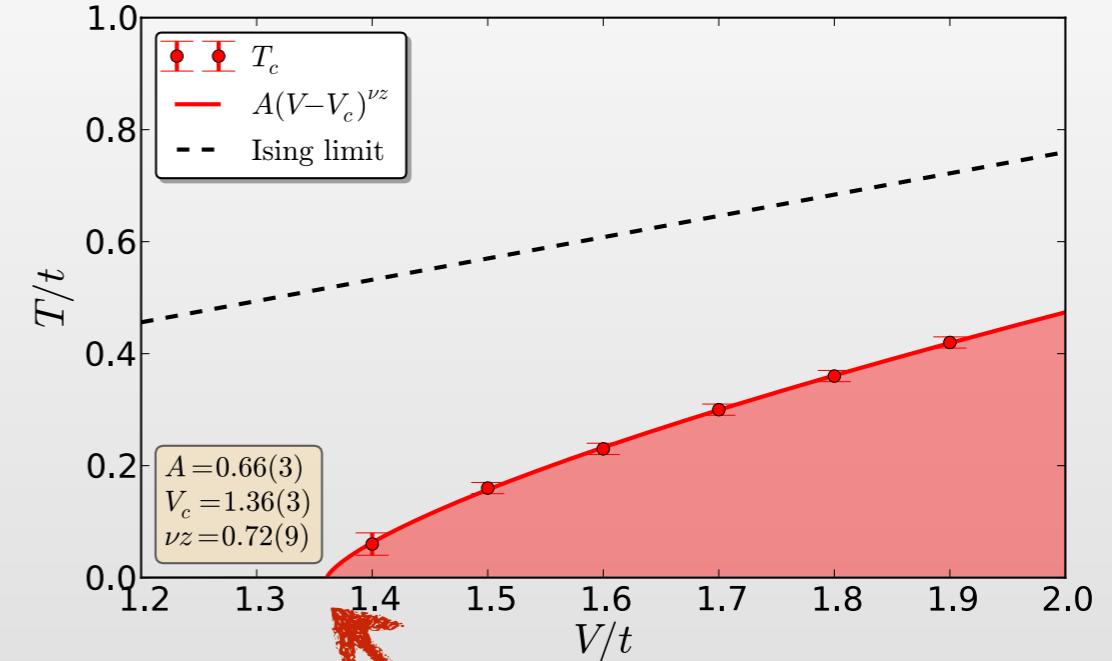
SU(3)

Solutions to the spinless t-V model

$$\hat{H}_0 = -t \sum_{\langle i,j \rangle} \left(\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_i \right)$$

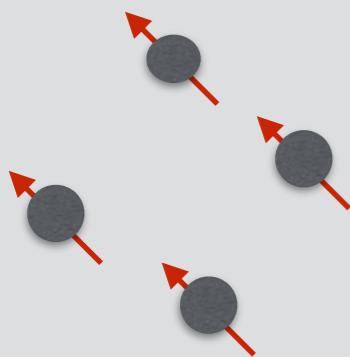
$$\hat{H}_1 = \frac{V}{4} \sum_{\langle i,j \rangle} \left(e^{i\pi(\hat{n}_i + \hat{n}_j)/2} \right) \left(\hat{n}_j - \frac{1}{2} \right)$$

$$w(\mathcal{C}_k) \sim \text{Tr} \left[(-1)^k e^{-(\beta - \tau_k) \hat{H}_0} \hat{H}_1 \dots \hat{H}_1 e^{-\tau_1 \hat{H}_0} \right]$$



Novel fermionic quantum critical point

see also Li, Jiang, Yao 2015 Hesselmann and Wessel 2016



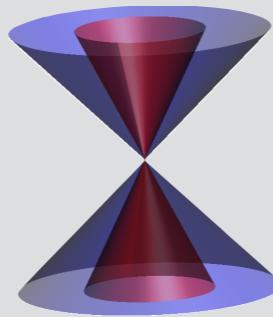
spinless fermions

LW, Troyer, PRL 2014

LW, Corboz, Troyer, NJP 2014

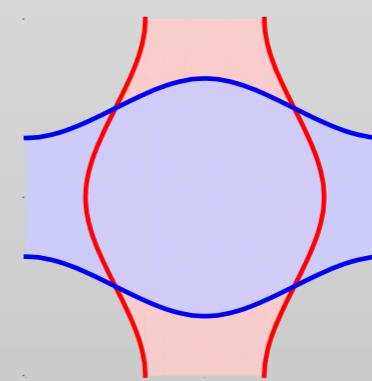
LW, Iazzi, Corboz, Troyer, PRB, 2015

LW, Liu and Troyer, PRB 2016

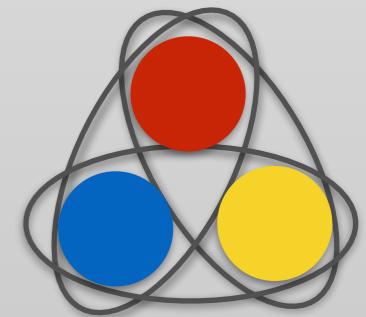


mass imbalance

Liu and LW, PRB 2015

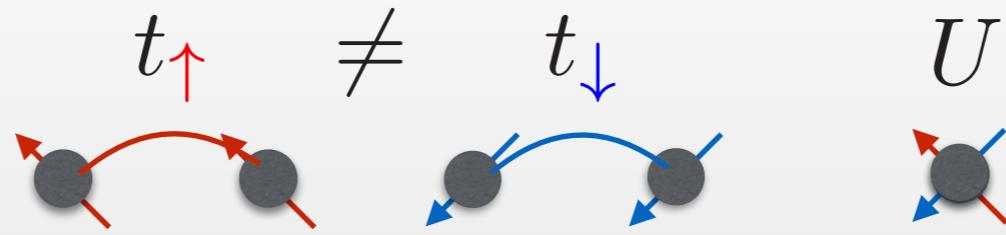


spin nematicity



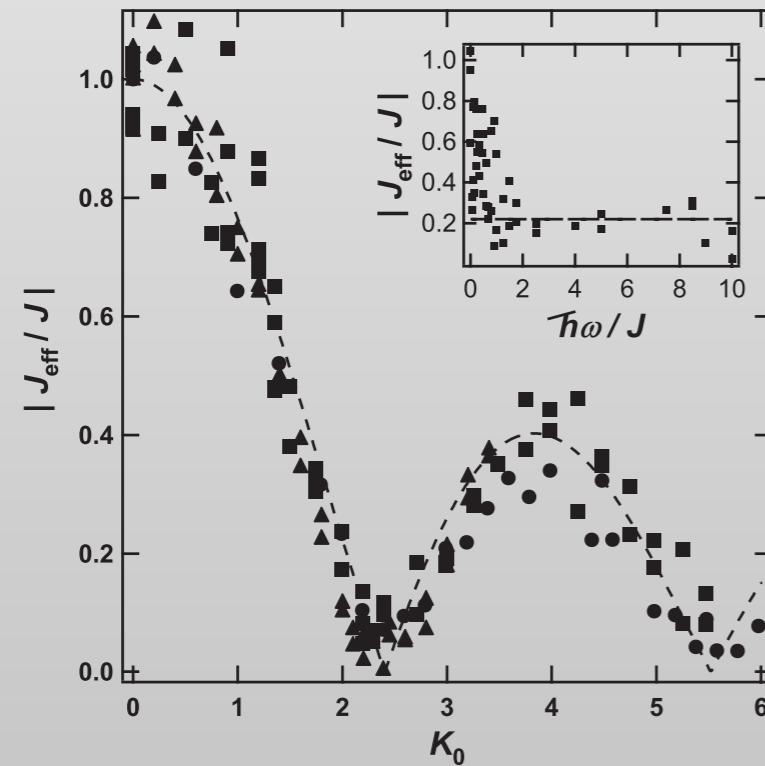
SU(3)

Asymmetric Hubbard model

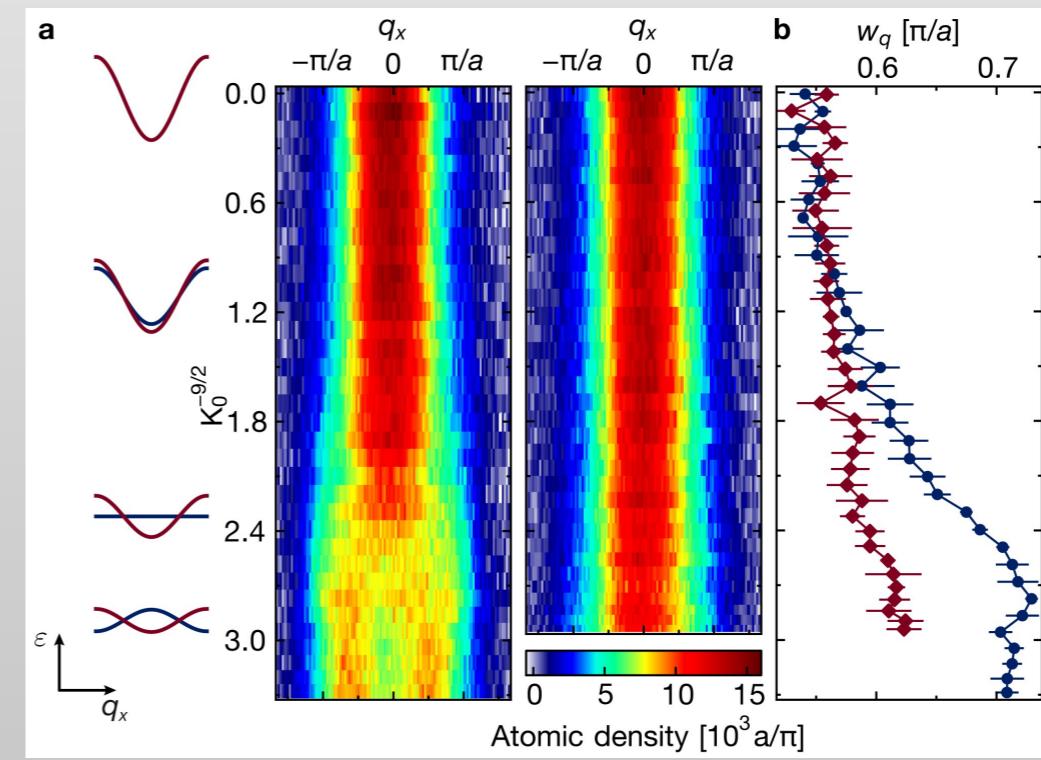


- Realization: mixture of ultracold fermions (e.g. ${}^6\text{Li}$ and ${}^{40}\text{K}$)
- Now, continuously tunable by **spin-dependent modulations**

$$t_{\downarrow}/t_{\uparrow} \in (-\infty, \infty)$$

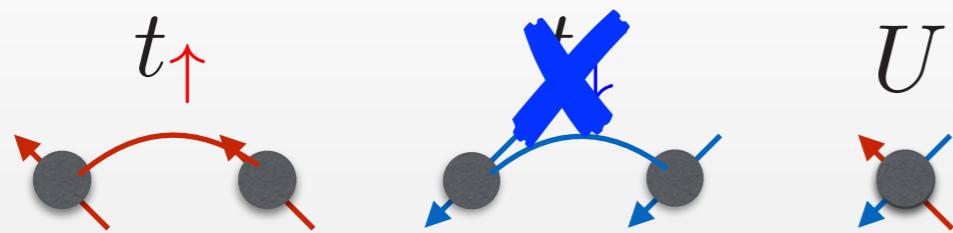


Lignier et al, PRL 2007 and many others



Jotzu et al, PRL 2015

Two limiting cases



Falicov-Kamball Limit

SIMPLE MODEL FOR SEMICONDUCTOR-METAL TRANSITIONS:
 SmB_6 AND TRANSITION-METAL OXIDES

L. M. Falicov*

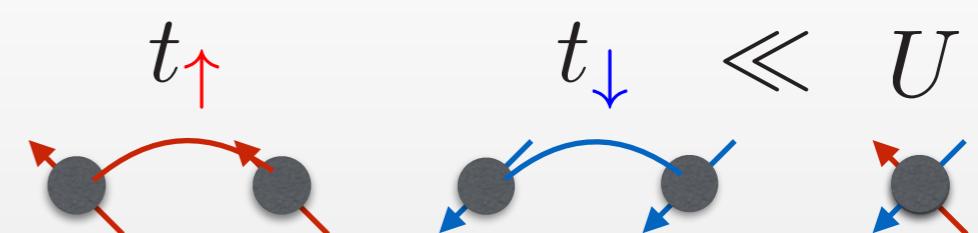
Department of Physics, University of California, Berkeley, California 94720

and

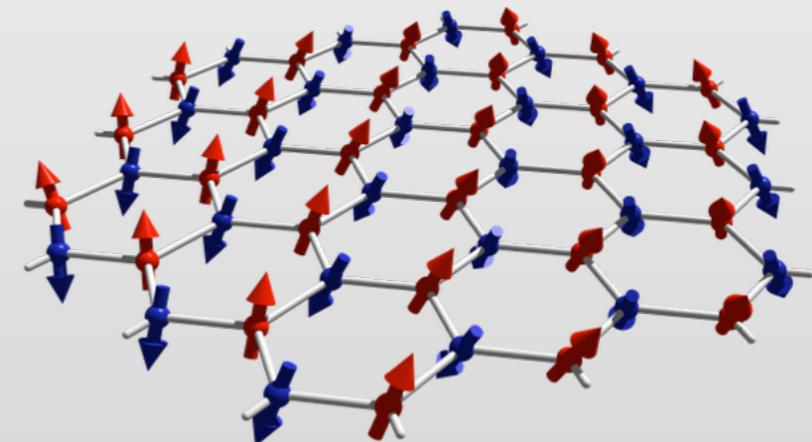
J. C. Kimball†

Department of Physics, and The James Franck Institute, University of Chicago, Chicago, Illinois 60637
(Received 12 March 1969)

We propose a simple model for a semiconductor-metal transition, based on the existence of both localized (ionic) and band (Bloch) states. It differs from other theories in that we assume the one-electron states to be essentially unchanged by the transition. The electron-hole interaction is responsible for the anomalous temperature dependence of the number of conduction electrons. For interactions larger than a critical value, a first-order semiconductor-metal phase transition takes place.



Strong Coupling Limit



$$J_{xy} (\hat{S}_i^x \hat{S}_j^x + \hat{S}_i^y \hat{S}_j^y) + J_z \hat{S}_i^z \hat{S}_j^z$$

$\frac{4t_\uparrow t_\downarrow}{U} \leq \frac{2(t_\uparrow^2 + t_\downarrow^2)}{U}$

Long-range spin order on bipartite lattices with infinitesimal repulsion

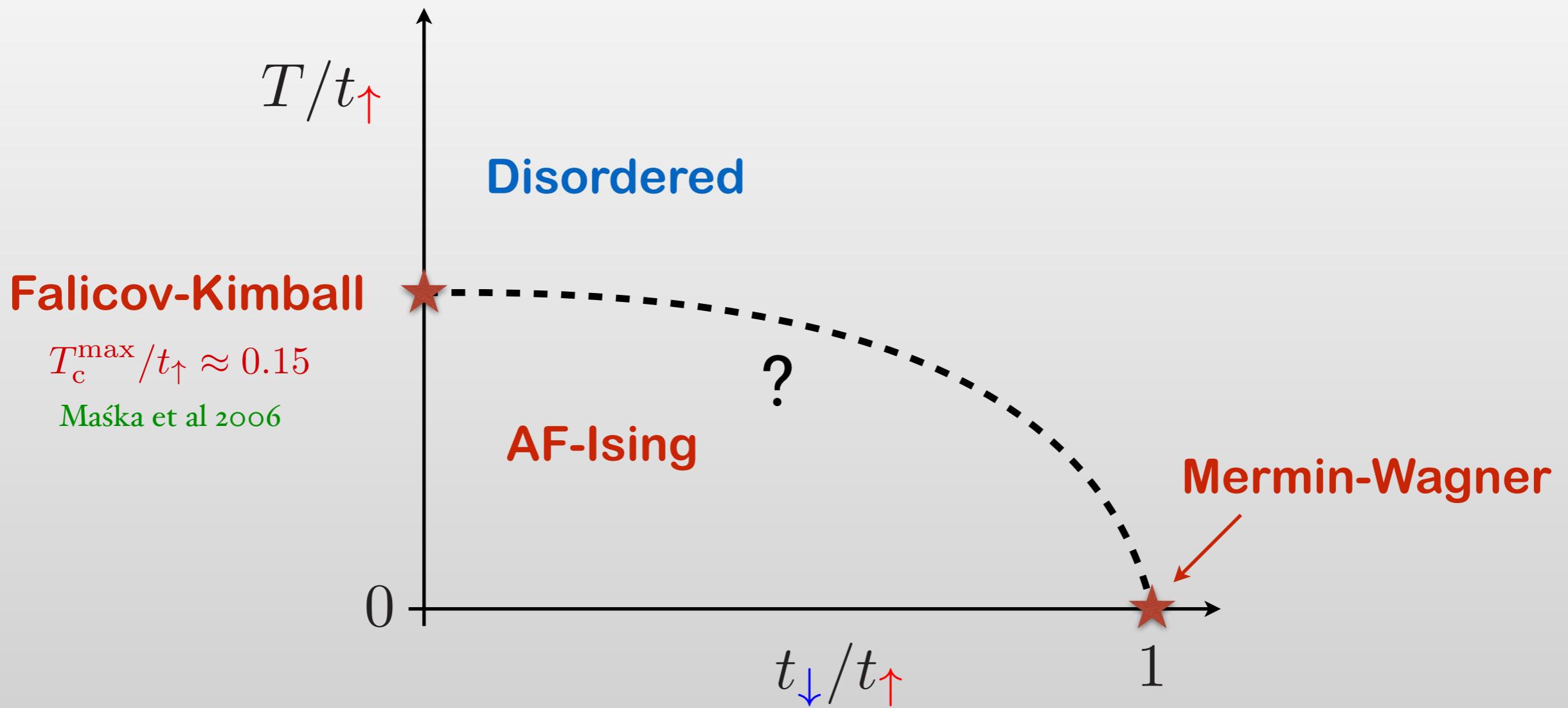
Kennedy and Lieb 1986

“Fruit fly” of DMFT

Freericks and Zlatić, RMP, 2003

XXZ model with Ising anisotropy

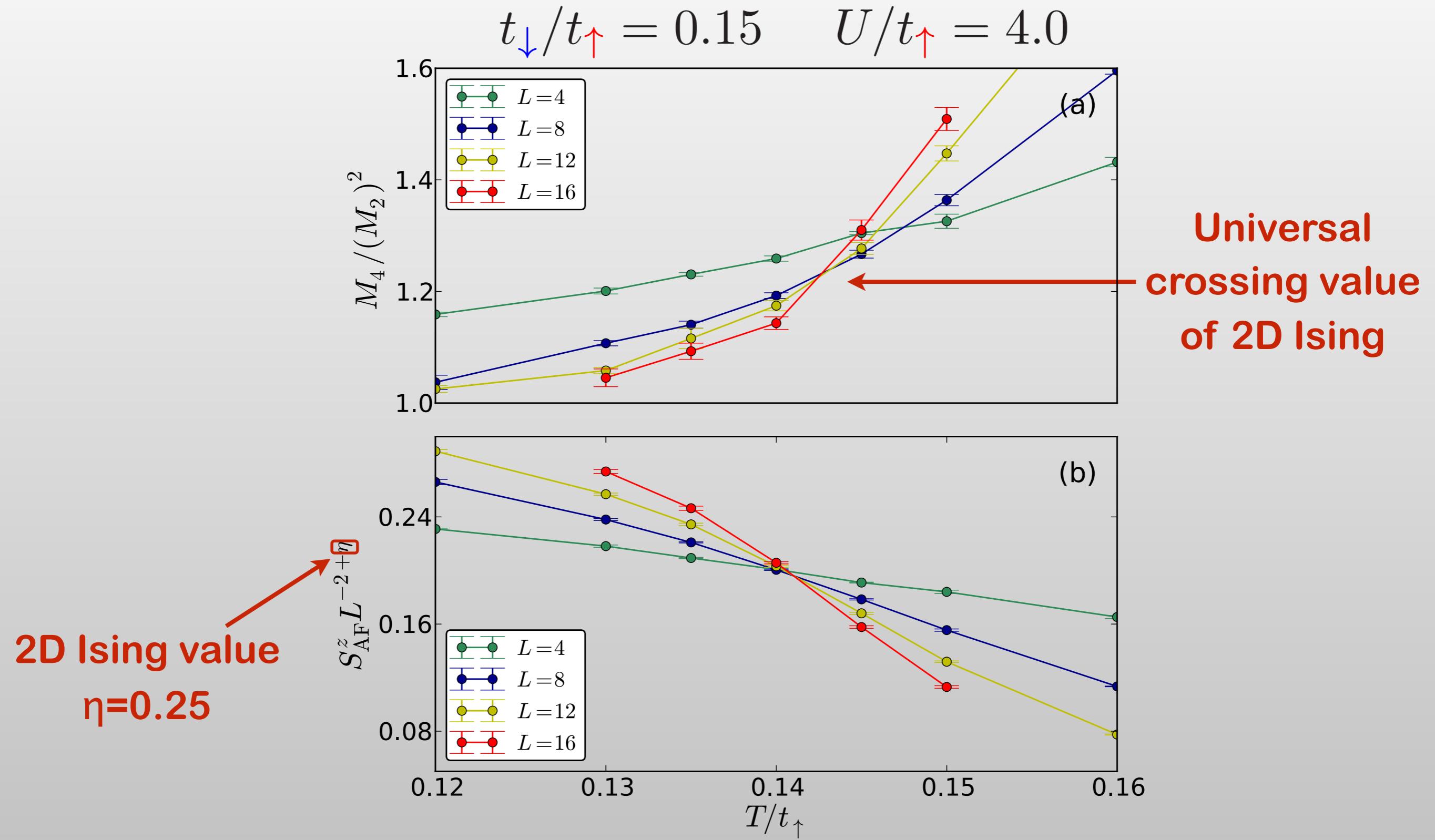
Physics on a square lattice



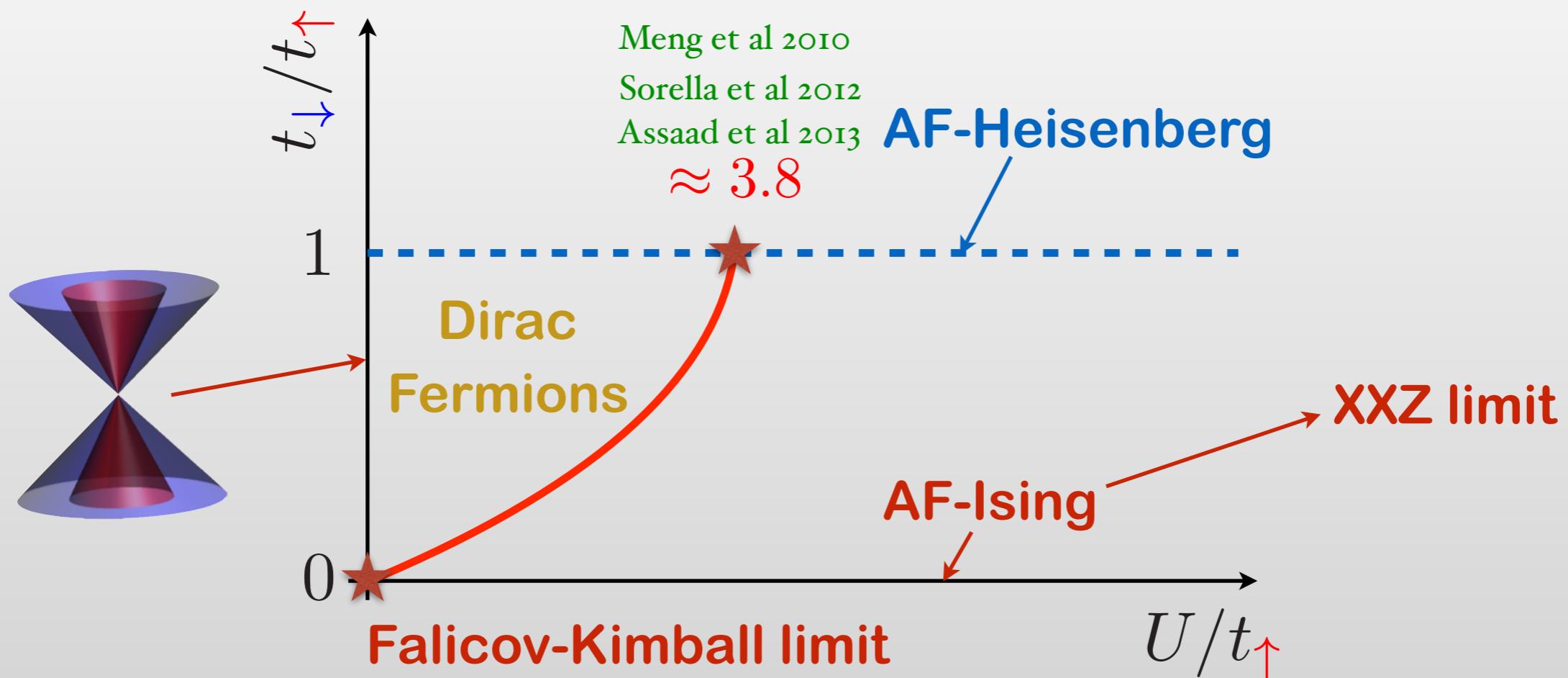
- Finite T_c in 2D because of broken Z_2 symmetry
- Advantage in 3D? Sotnikov et al, PRL 2012

Locate the critical temperature

Liu and LW, PRB 2015



Physics on a honeycomb lattice

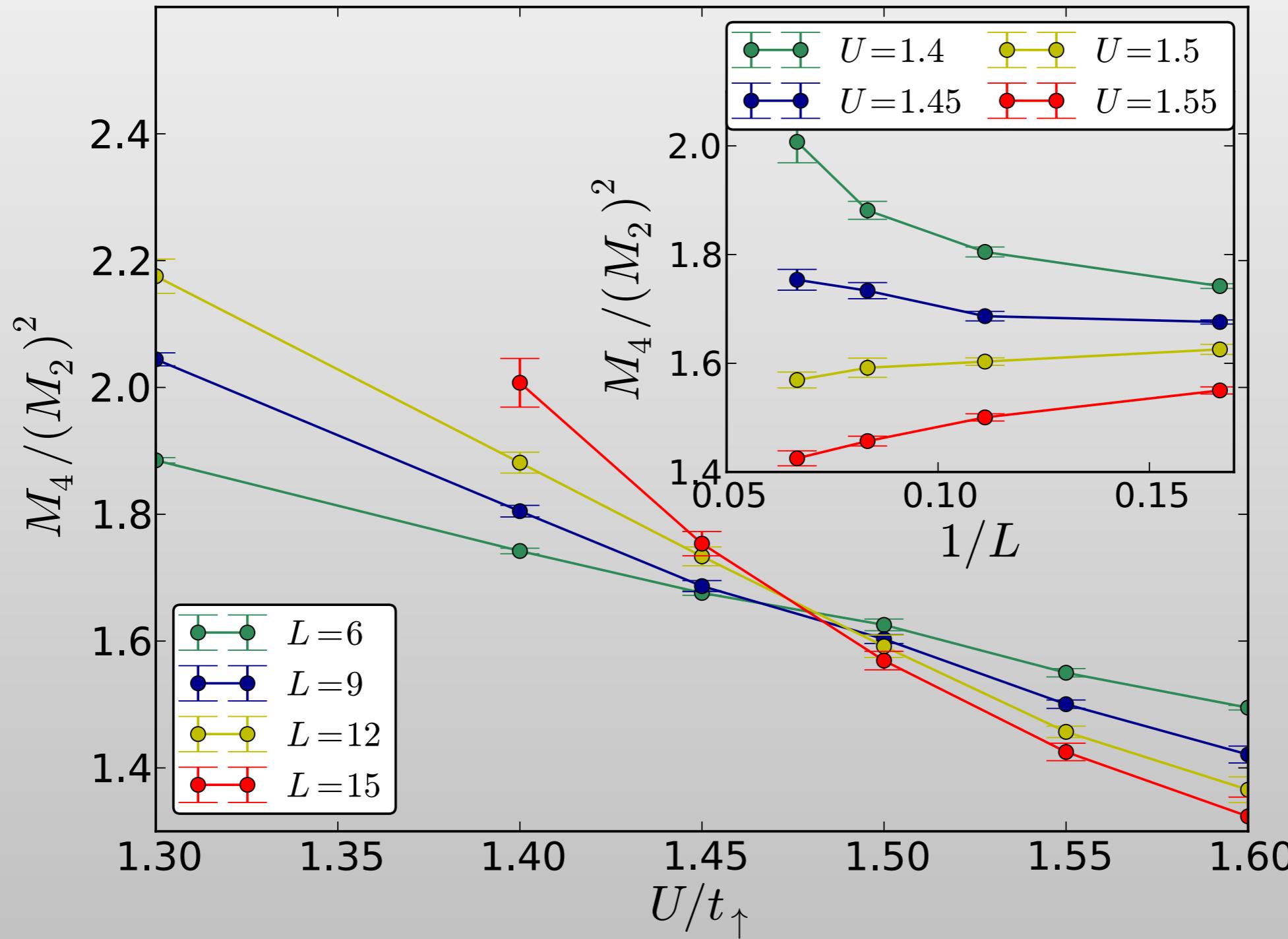


- 📌 How to connect the phase boundary ?
- 📌 What is the universality class ?

Binder ratio

$t_{\downarrow}/t_{\uparrow} = 0.15$

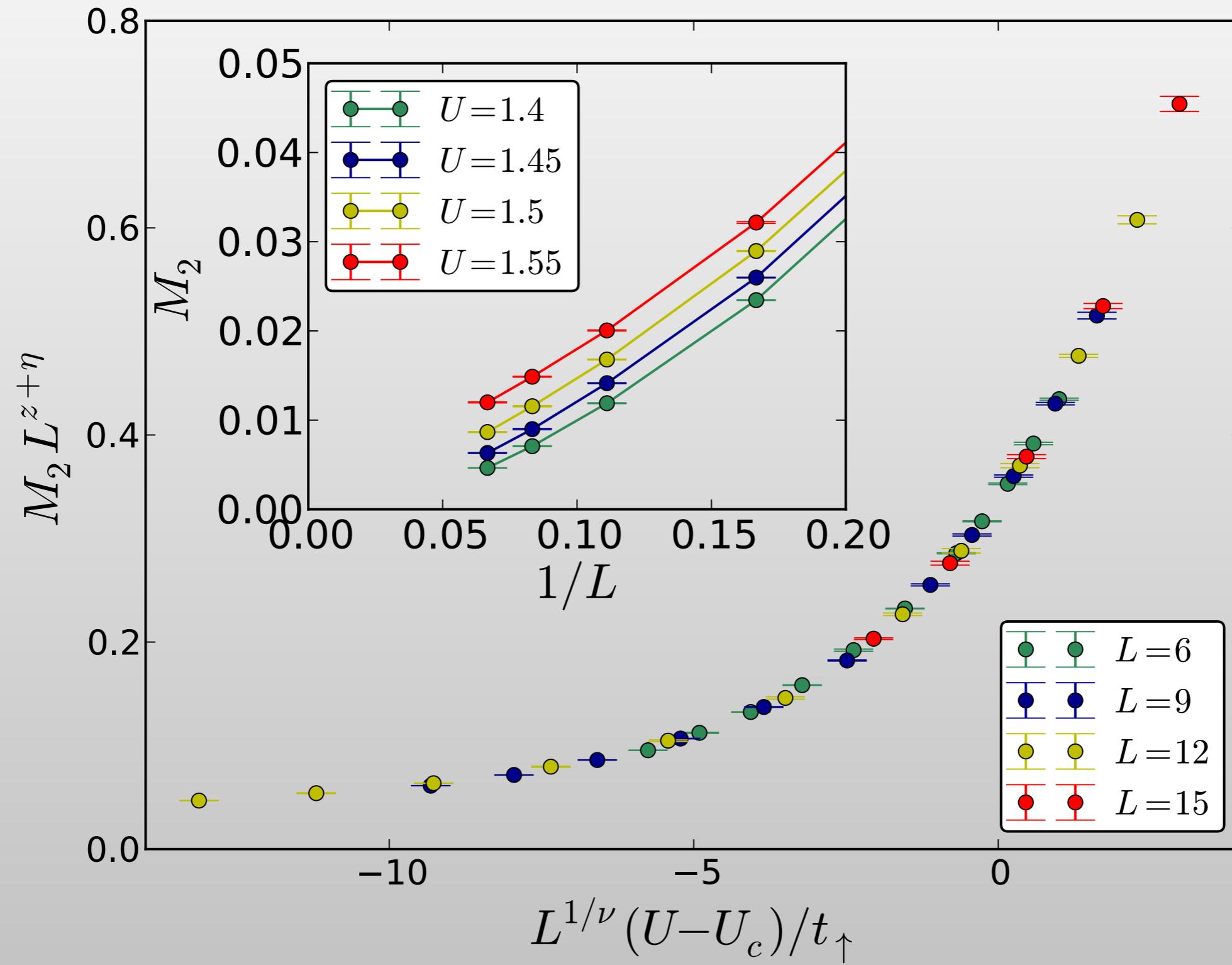
$$M_2 = \left\langle \left(\frac{1}{N} \sum_{\mathbf{r}} e^{i\mathbf{Q} \cdot \mathbf{r}} \frac{\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow}}{2} \right)^2 \right\rangle \quad M_4 = \left\langle \left(\frac{1}{N} \sum_{\mathbf{r}} e^{i\mathbf{Q} \cdot \mathbf{r}} \frac{\hat{n}_{\mathbf{r}\uparrow} - \hat{n}_{\mathbf{r}\downarrow}}{2} \right)^4 \right\rangle$$



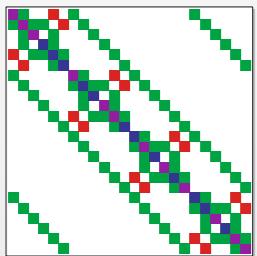
Scaling analysis

$\nu = 0.84(4)$

$z + \eta = 1.395(7)$



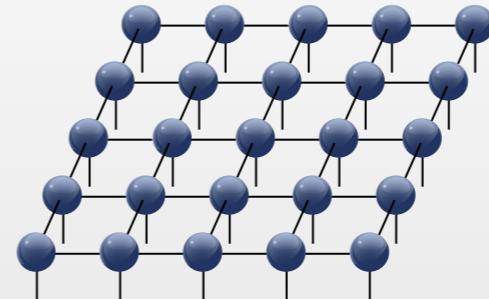
Summary



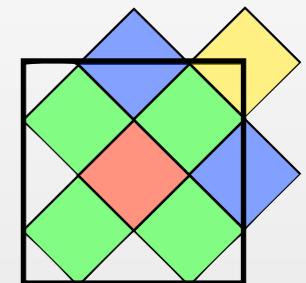
exact
diagonalization



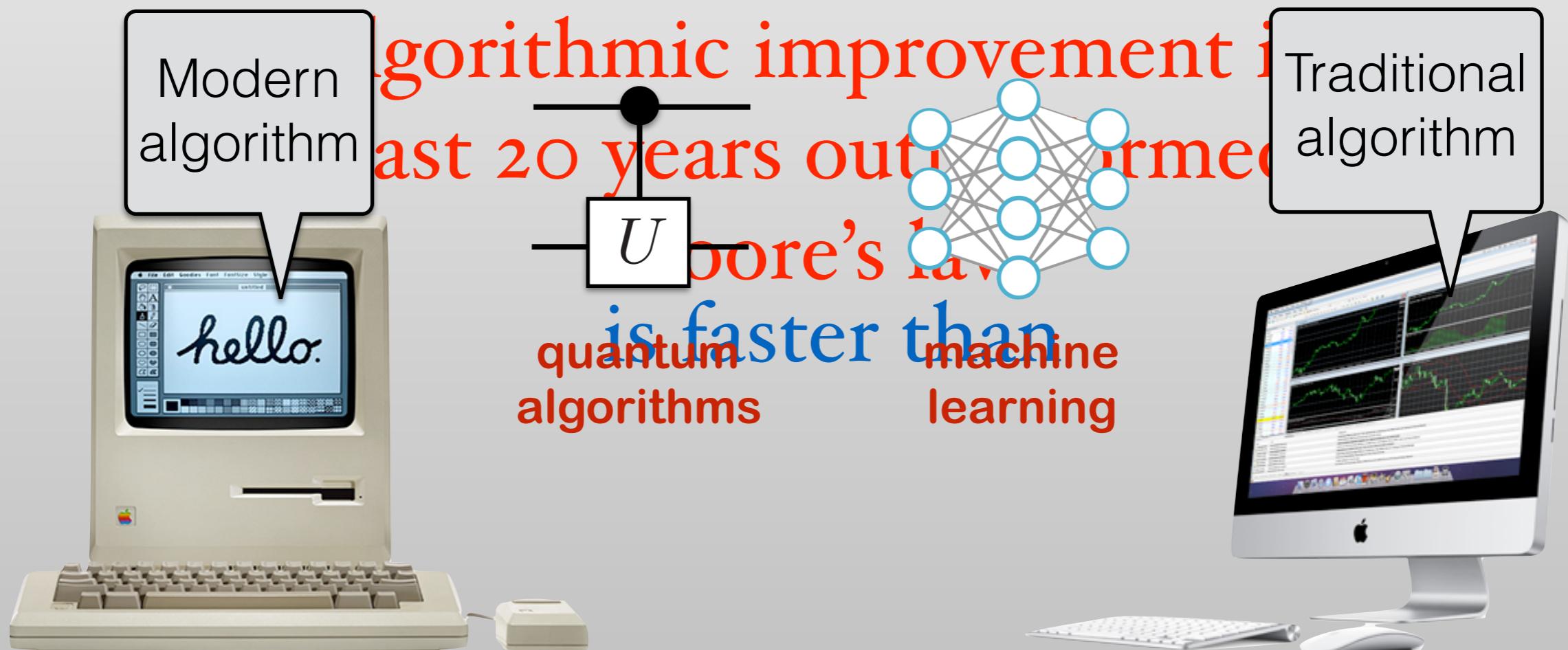
quantum
Monte Carlo



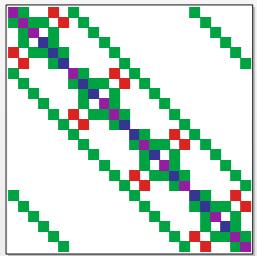
tensor network
states



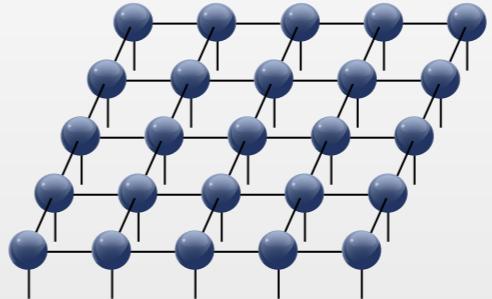
dynamical mean
field theories



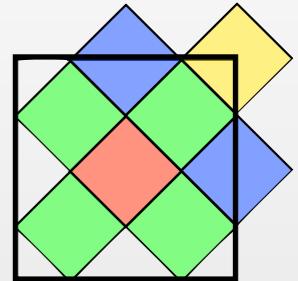
Summary



exact
diagonalization



tensor network
states



dynamical mean
field theories

Thanks to my collaborators!

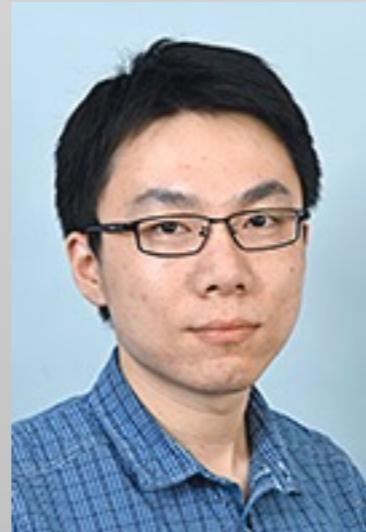
Hsiang-Hsuan
Hung



Gergely
Harcos



Ye-Hua
Liu



Mauro
Iazzi

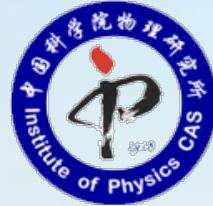


Philippe
Corboz



Matthias
Troyer





中国科学院物理研究所
Institute of Physics Chinese Academy of Sciences

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